Electronic Supplementary Material (ESI) for Chemical Communications.

Ferrocene/Air Double-Mediated $FeTiO_3$-Photocatalyzed Semi-heterogeneous Annulation of Quinoxalin-2(1*H*)-ones in EtOH/H_2O

Wen-Tao Ouyang[a], Hong-Tao Ji[a], Jun Jiang[a], Chao Wu[a], Jia-Chen Hou[a], Min-Hang Zhou[a], Yu-Han Lu[a], Li-Juan Ou[b]*, Wei-Min He[a]*

School of Chemistry and Chemical Engineering, University of South China, Hengyang, 421001, China

Wei-Min He: weiminhe@usc.edu.cn

oulijuanann@163.com

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1. General Information

Unless otherwise specified, all reagents and solvents were obtained from commercial suppliers and used without further purification. ^{1}H NMR spectra were recorded at 500 MHz, ^{13}C NMR spectra were recorded at 126 MHz and ^{19}F NMR spectra were recorded at 471 MHz by using a Bruker Avance 500 spectrometer. Chemical shifts were calibrated using residual undeuterated solvent as an internal reference (^{1}H NMR: $CDCl_3$ 7.26 ppm； dmso-d6 2.50ppm, ^{13}C NMR: $CDCl_3$ 77.16 ppm；dmso-d6 39.52ppm), the chemical shifts (δ) were expressed in ppm and J values were given in Hz. The following abbreviations were used to describe peak splitting patterns when appropriate: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, br = broad. Mass spectra were performed on a spectrometer operating on ESI-TOF. Powder X-ray diffraction (PXRD) data were collected on a Rigaku Smartlab 9 kW X-ray diffractometer operating at 45 kV/200mA using the Cu Ka line (λ = 1.5418 Å). PXRD patterns were measured over the 20 range of 3-50 with 5 per min per step over 10 min. Column chromatography was performed on silica gel (200-300 mesh). The gram-scale synthesis crude products were purified by HPLC (LaboACE LC-5060, Japan Analytical Industry Co., Ltd., Japan) equipped with Jaigel 2.5 HR columns with dichloromethane as the eluent.

The Light Source and the Material of the Irradiation Vessel

Manufacturer：Beijing Rogertech Ltd.

Model：OHSP-350 UV

Value: 2662.138 μW/cm²/nm

Energy peak wavelength：516.0 nm

Peak width at half-height：22.1 nm

Material of the irradiation vessel：Schlenk flask

Not use any filters

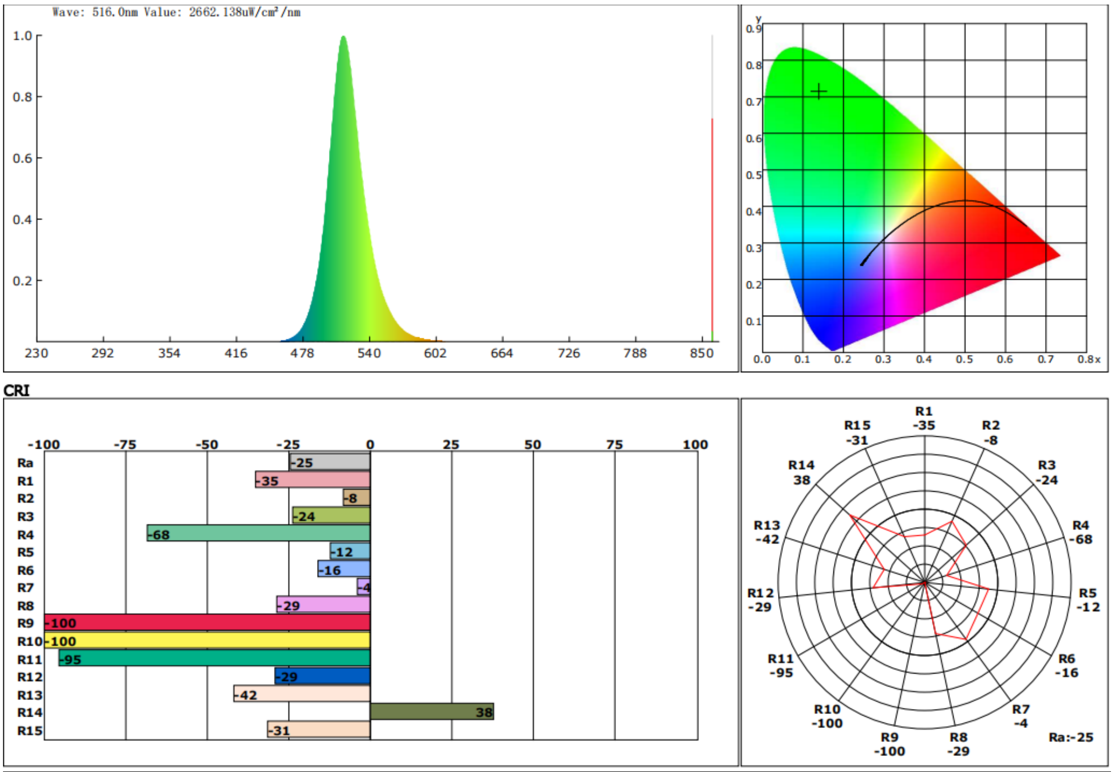


Figure S1：LED spectrum test report

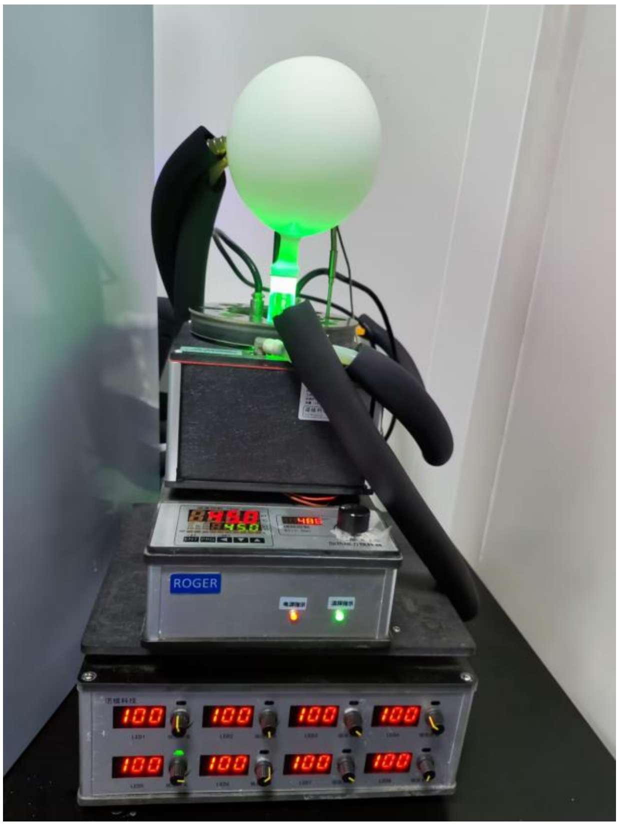
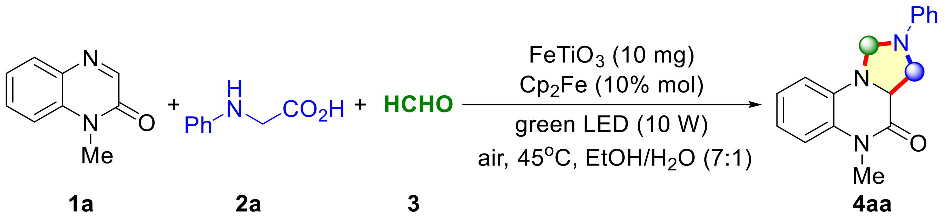


Figure S2（Photographed by author Wen-Tao Ouyang）

2. Experimental Section

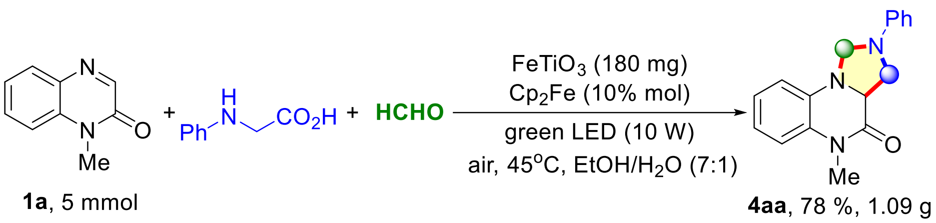
2.1 General Procedure for Compounds 4aa



Scheme S1

To a solution of 1-methylquinoxalin-2(1*H*)-one **1a** (0.2 mmol) in EtOH (3.15 mL) and H_2O (0.45 mL) was added *N*-phenyglycine **2a** (0.24 mmol), formaldehyde **3** (0.24 mmol), $FeTiO_3$ (10 mg) and Cp_2Fe (0.02 mmol). The reaction mixture was equip with an air balloon and stirred at 45 °C under the irradiation of green LED (10 W) for 2 h. After completion, the solvent was concentrated under reduced pressure, and the pure products **4aa** was obtained by flash chromatography on silica gel.

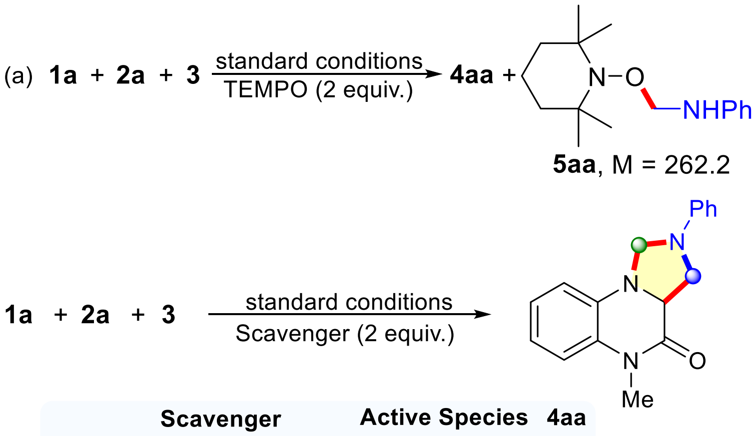
2.2 Gram-scale synthesis of 4aa



Scheme S2

To a solution of 1-methylquinoxalin-2(1*H*)-one **1a** (5 mmol) in EtOH (21 mL) and H_2O (3 mL) was added *N*-phenylglycine **2a** (6 mmol), formaldehyde **3** (6 mmol), $FeTiO_3$ (180 mg) and Cp_2Fe (0.5 mmol)，The reaction mixture was equip with an air balloon and stirred at 45 °C under the irradiation of green LED (10 W). After completion of the reaction, the resulting mixture was filtrated and the organic phase was removed under vacuum. The residue was purified by HPLC to give 1.09 gram of **4aa**, 78% yield.

2.3 Radical Trapped Experiments



	Scavenger	Active Species	4aa
(b)	1,4-benzoquinone	$O_2^{\bullet-}$	22%
(c)	isopropanol	$HO^{\bullet}$	84%
(d)	9,10-diphenylanthracene	$^1O_2$	77%
(e)	$FeSO_4$	$HOO^{\bullet}$	86%
(f)	Na_2S	Hole	trace
(g)	$AgNO_3$	e^-	trace
(h)	1,4-dinitrobenzene	SET	trace

Scheme S3

(a) To a solution of 1-methylquinoxalin-2(1*H*)-one **1a** (0.2 mmol) in EtOH (3.15 mL) and H_2O (0.45 mL) was added *N*-phenylglycine **2a** (0.24 mmol), formaldehyde **3** (0.24 mmol), $FeTiO_3$ (10 mg), Cp_2Fe (0.02 mmol) and TEMPO (0.4 mmol). The reaction mixture was equipped with an air balloon and stirred at 45 °C under the irradiation of green LED (10 W) for about 2 h. The reaction mixture was analyzed by GC and a trace amount of **4aa** was detected.

(b) To a solution of 1-methylquinoxalin-2(1*H*)-one **1a** (0.2 mmol) in EtOH (3.15 mL) and H_2O (0.45 mL) was added *N*-phenylglycine **2a** (0.24 mmol), formaldehyde **3** (0.24 mmol), $FeTiO_3$ (10 mg), Cp_2Fe (0.02 mmol) and 1,4-benzoquinone (0.4 mmol). The reaction mixture was equipped with an air balloon and stirred at 45 °C under the irradiation of green LED (10 W) for about 2 h. The reaction mixture was analyzed by GC and a 22% yield of **4aa** was detected.

(c) To a solution of 1-methylquinoxalin-2(1*H*)-one **1a** (0.2 mmol) in EtOH (3.15 mL) and H_2O (0.45 mL) was added *N*-phenylglycine **2a** (0.24 mmol), formaldehyde **3** (0.24 mmol), $FeTiO_3$ (10 mg), Cp_2Fe (0.02 mmol) and isopropanol (0.4 mmol). The reaction mixture was equipped with an air balloon and stirred at 45 °C under the irradiation of green LED (10 W) for about 2 h. The reaction mixture was analyzed by GC and an 84% yield amount of **4aa** was detected.

(d) To a solution of 1-methylquinoxalin-2(1*H*)-one **1a** (0.2 mmol) in EtOH (3.15 mL) and H_2O (0.45 mL) was added *N*-phenylglycine **2a** (0.24 mmol), formaldehyde **3** (0.24 mmol), $FeTiO_3$ (10 mg), Cp_2Fe (0.02 mmol) and 9,10-diphenylanthracene (0.4 mmol). The reaction mixture was equipped with an air balloon and stirred at 45 ℃ under the irradiation of green LED (10 W) for about 2 h. The reaction mixture was analyzed by GC and an 77% yield of **4aa** was detected.

(e) To a solution of 1-methylquinoxalin-2(1*H*)-one **1a** (0.2 mmol) in EtOH (3.15 mL) and H_2O (0.45 mL) was added *N*-phenylglycine **2a** (0.24 mmol), formaldehyde **3** (0.24 mmol), $FeTiO_3$ (10 mg), Cp_2Fe (0.02 mmol) and $FeSO_4$ (0.4 mmol). The reaction mixture was equipped with an air balloon and stirred at 45 ℃ under the irradiation of green LED (10 W) for about 2 h. The reaction mixture was analyzed by GC and an 86% yield of **4aa** was detected.

(f) To a solution of 1-methylquinoxalin-2(1*H*)-one **1a** (0.2 mmol) in EtOH (3.15 mL) and H_2O (0.45 mL) was added *N*-phenylglycine **2a** (0.24 mmol), formaldehyde **3** (0.24 mmol), $FeTiO_3$ (10 mg), Cp_2Fe (0.02 mmol) and Na_2S (0.4 mmol). The reaction mixture was equipped with an air balloon and stirred at 45 ℃ under the irradiation of green LED (10 W) for about 2 h. The reaction mixture was analyzed by GC and a trace amount of **4aa** was detected.

(g) To a solution of 1-methylquinoxalin-2(1*H*)-one **1a** (0.2 mmol) in EtOH (3.15 mL) and H_2O (0.45 mL) was added *N*-phenylglycine **2a** (0.24 mmol), formaldehyde **3** (0.24 mmol), $FeTiO_3$ (10 mg), Cp_2Fe (0.02 mmol) and $AgNO_3$ (0.4 mmol). The reaction mixture was equipped with an air balloon and stirred at 45 ℃ under the irradiation of green LED (10 W) for about 2 h. The reaction mixture was analyzed by GC and a trace amount of **4aa** was detected.

(h) To a solution of 1-methylquinoxalin-2(1*H*)-one **1a** (0.2 mmol) in EtOH (3.15 mL) and H_2O (0.45 mL) was added *N*-phenylglycine **2a** (0.24 mmol), formaldehyde **3** (0.24 mmol), $FeTiO_3$ (10 mg), Cp_2Fe (0.02 mmol) and 1,4-dinitrobenzene (0.4 mmol). The reaction mixture was equipped with an air balloon and stirred at 45 ℃ under the irradiation of green LED (10 W) for about 2 h. The reaction mixture was analyzed by GC and a trace amount of **4aa** was detected.

2.4 Reusability and Stability of Photocatalyst

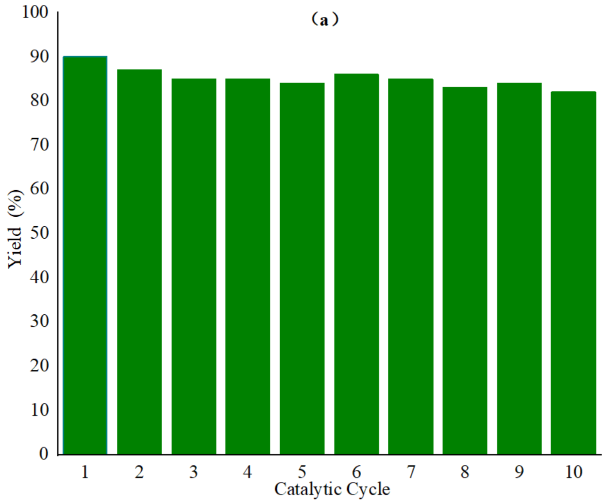


Figure S3 Reusability and Stability of Photocatalyst

To a solution of 1-methylquinoxalin-2(1*H*)-one **1a** (0.2 mmol) in EtOH (3.15 mL) and H_2O (0.45 mL) was added *N*-phenylglycine **2a** (0.24 mmol), formaldehyde **3** (0.24 mmol), $FeTiO_3$ (10mg), Cp_2Fe (0.02 mmol). The reaction mixture was equipped with an air balloon and stirred at 45 °C under the irradiation of green LED (10 W) for about 2 h. After completion of the reaction, the photocatalyst was separated by centrifugation, washed twice with EtOH and used for next run. The reaction mixture was analysed by GC to give the yield of **4aa.**

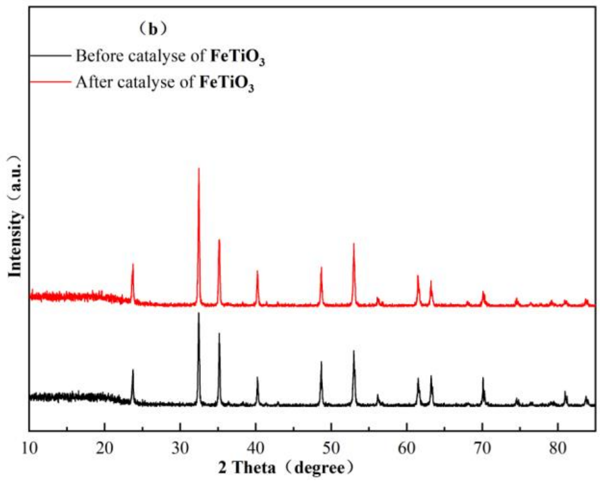


Figure S4 XRD patterns of fresh $FeTiO_3$ and recycled $FeTiO_3$.

2.5 Effect of Visible Light Irradiation

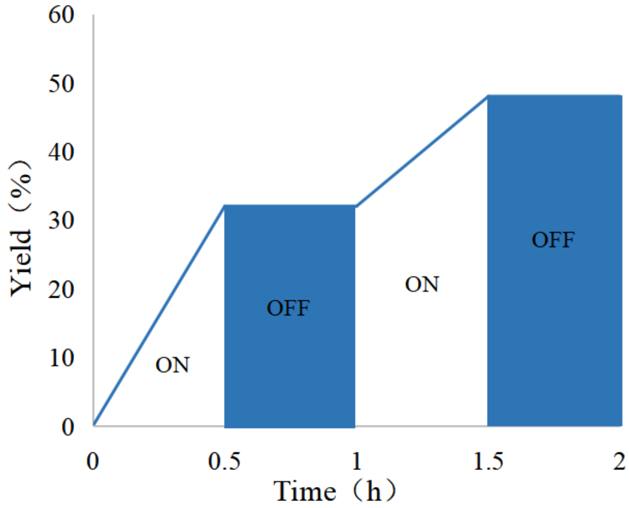


Figure S5 Effect of Visible Light Irradiation

The model reaction was conducted under the standard conditions on a 0.2 mmol scale. The mixture was subjected to sequential periods of stirring under green LED (10 W) irradiation followed by stirring in the absence of light. At each time point, one reaction system was suspended and the yield was detected by GC.

2.6 Cyclic Voltammetry Experiments

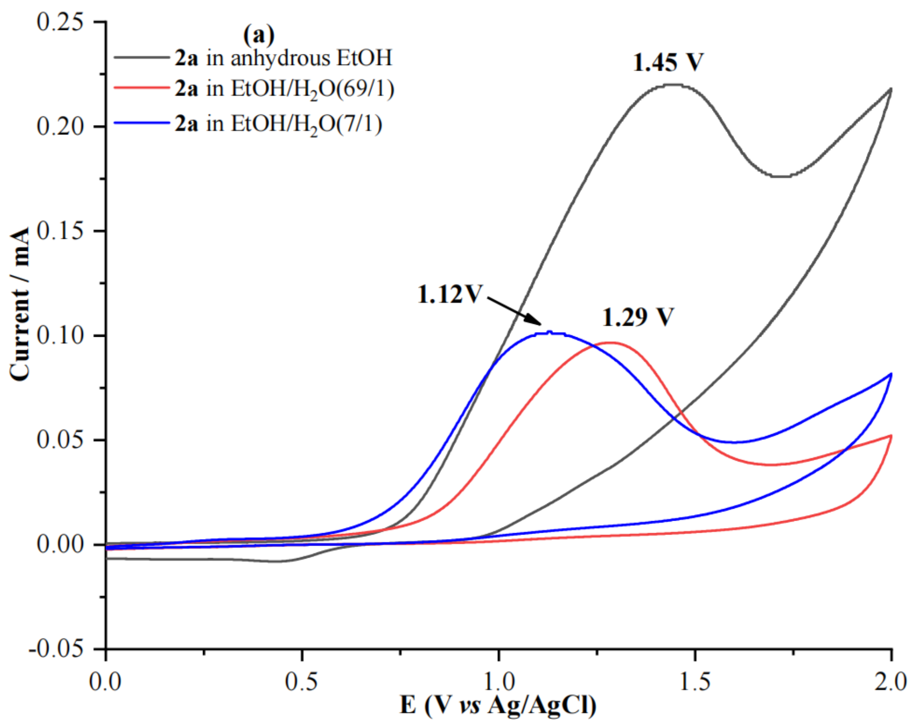


Figure S6. Cyclic voltammogram experiments of $^nBu_4BF_4N$ (0.1 M) as electrolyte in anhydrous EtOH or EtOH/H_2O from 0 V to +2.0 V at room temperature

The CV measurements were performed on a CHI 660E potentiostat, and the conditions are as follow: a glassy carbon disk working electrode (diameter, 3 mm), Pt disk and Ag/AgCl as counter and reference electrode. As shown in the Figure S4, $^nBu_4BF_4N$ (0.1 M) as electrolyte in 10 mL anhydrous EtOH or EtOH/H_2O. And cyclic voltammograms of reactants and their mixtures in 0.1 M $^nBu_4BF_4N$ glassy carbon disk working electrode (diameter, 3 mm), Pt disk and Ag/AgCl (0.1 M in anhydrous EtOH or EtOH/H_2O) as counter and reference electrode at 100 mV/s scan rate: (1) 10 mM **2a** in anhydrous EtOH (10 mL) (black line), (2) 10 mM **2a** in EtOH/H_2O (69/1) (10 mL) (red line), (3)10 mM **2a** in EtOH/H_2O (7/1) (10 mL) (blue line)

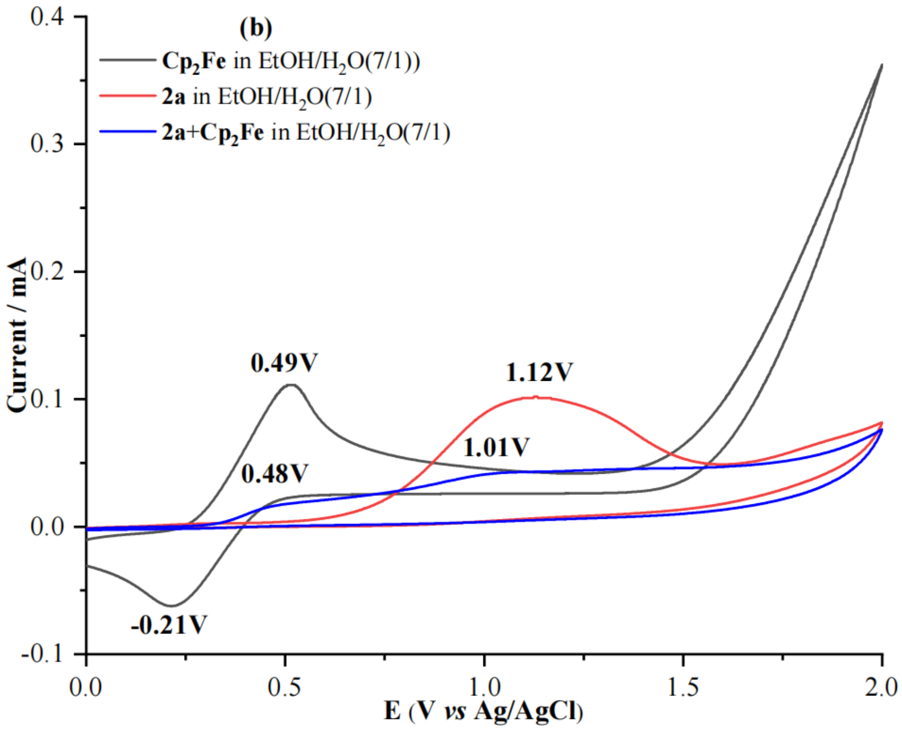


Figure S7 Cyclic voltammogram experiments of $^nBu_4BF_4N$ (0.1 M) as electrolyte in EtOH/H_2O (7/1) from 0 V to +2.0 V at room temperature

As shown in the Figure S7, $^nBu_4BF_4N$ (0.1 M) as elctrolyte in 10 mL anhydrous EtOH/H_2O (7/1). And cyclic voltammograms of reactants and their mixtures in glassy carbon disk working electrode (diameter, 3 mm), Pt disk and Ag/AgCl (0.1 M in EtOH/H_2O (7/1)) as counter and reference electrode at 100 mV/s scan rate: (1) 10 mM

Cp_2Fe in EtOH/H_2O (7/1) (black line), (2) 10 mM **2a** in EtOH/H_2O (7/1) (red line), (3) 10 mM **2a** and Cp_2Fe in EtOH/H_2O (7/1) (blue line)。

2.7 Fe^{3+} verification experiment

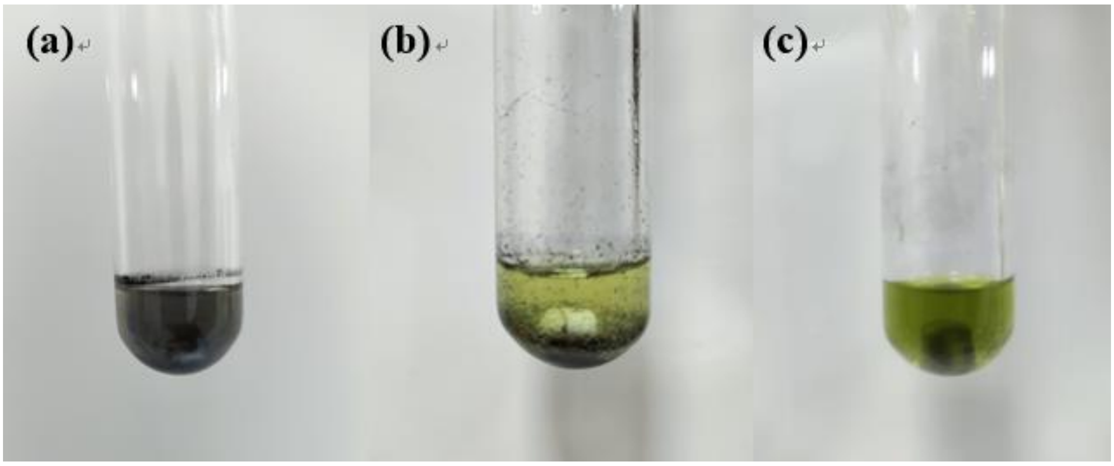
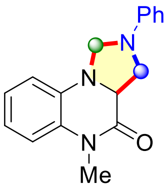


Figure S8 Fe^{3+} verification experiment

As shown in the Figure S8 (a) $K_4Fe(CN)_6$ (0.1 mmol), **1a** (0.1 mmol), $FeTiO_3$ (20 mg) in 2 mL EtOH/H_2O (1/1). (b) $K_4Fe(CN)_6$ (0.1 mmol), **1a** (0.1 mmol), $FeTiO_3$ (20 mg) in 2 mL EtOH/H_2O (1/1), The reaction mixture was equip with an air balloon and stirred at 45 °C under the irradiation of green LED (10 W) for about 60 min. (c) $K_3Fe(CN)_6$ (0.05 mmol), **1a** (0.05 mmol), $FeTiO_3$ (10 mg) in 2 mL EtOH/H_2O (1/1).

3. Characterization Data for Products

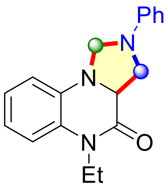
5-methyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one (4aa)[1]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 (t, J = 7.7 Hz, 2H), 7.03 (t, J = 7.5 Hz, 1H), 6.97 (d, J = 7.8 Hz, 1H), 6.92 (t, J = 7.6 Hz, 1H), 6.77 (t, J = 7.2 Hz, 1H), 6.58 (t, J = 7.5 Hz, 3H), 4.67 (d, J = 3.0 Hz, 1H), 4.56 (d, J = 2.9 Hz, 1H), 3.99 – 3.92 (m, 1H), 3.84 (t, J = 7.6 Hz, 1H), 3.68 (t, J = 8.8 Hz, 1H), 3.35 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.4, 145.7, 134.2, 130.3, 129.4, 124.0, 120.1, 117.4, 115.1, 112.0, 111.7, 64.6, 58.7, 48.5, 29.0.

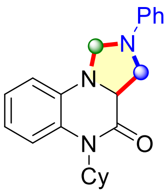
5-ethyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one(4ba)[1]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 (t, J = 7.8 Hz, 2H), 7.11 – 7.05 (m, 2H), 6.97 (t, J = 7.7 Hz, 1H), 6.81 (t, J = 7.3 Hz, 1H), 6.69 – 6.63 (m, 3H), 4.77 (d, J = 3.2 Hz, 1H), 4.64 (d, J = 3.2 Hz, 1H), 4.17 – 4.09 (m, 1H), 4.04 – 3.96 (m, 2H), 3.91 (t, J = 7.6 Hz, 1H), 3.78 (t, J = 8.8 Hz, 1H), 1.31 (t, J = 7.2 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.0, 145.8, 134.6, 129.5, 129.2, 124.0, 120.3, 117.5, 115.0, 112.4, 111.8, 64.7, 58.8, 48.5, 37.2, 12.8.

5-cyclohexyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one （4ca）

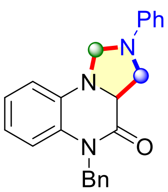


^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 (t, J = 7.4 Hz, 2H), 7.11 – 7.04 (m, 2H), 6.96 (t, J = 7.7 Hz, 1H), 6.80 (d, J = 7.2 Hz, 1H), 6.69 – 6.63 (m, 3H), 4.79 (d, J = 2.5 Hz, 1H), 4.67 – 4.61 (m, 1H), 4.07 – 3.99 (m, 2H), 3.91 (t, J = 7.6 Hz, 1H), 3.80 (d, J = 8.8 Hz, 1H), 1.81 – 1.67 (m, 5H), 1.21 – 1.07 (m, 5H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.7, 145.9, 134.8, 129.6, 129.6, 123.9, 120.2, 117.5, 115.7, 112.5, 111.8, 64.8, 58.8, 48.7, 47.4, 35.9, 31.1, 30.6, 26.4, 26.0.

HRMS (ESI) m/z calcd for $C_{22}H_{26}N_3O$ $[M+H]^+$： 348.2070, found 348.2068

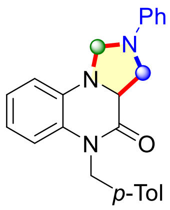
5-benzyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one(4da)[1]



^1H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.29 (m, 4H), 7.27 – 7.22 (m, 3H), 7.03 (t, J = 7.6 Hz, 1H), 6.93 (d, J = 8.0 Hz, 1H), 6.84 – 6.78 (m, 2H), 6.65 (d, J = 7.7 Hz, 3H), 5.44 (d, J = 16.2 Hz, 1H), 4.97 (d, J = 16.2 Hz, 1H), 4.80 (d, J = 3.2 Hz, 1H), 4.67 (d, J = 3.1 Hz, 1H), 4.19 – 4.13 (m, 1H), 3.96 (t, J = 7.7 Hz, 1H), 3.84 (t, J = 8.9 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.8, 145.8, 136.5, 134.6, 129.7, 129.6, 128.9, 127.4, 126.6, 124.2, 120.4, 117.6, 116.1, 112.3, 111.8, 64.8, 59.0, 48.6, 45.9.

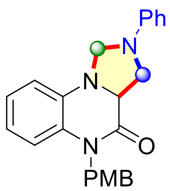
5-(4-methylbenzyl)-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one(4ea)[1]



^1H NMR (500 MHz, $CDCl_3$) δ 7.34 (t, J = 7.6 Hz, 2H), 7.21 – 7.13 (m, 4H), 7.06 (t, J = 7.6 Hz, 1H), 6.98 (d, J = 8.0 Hz, 1H), 6.88 – 6.82 (m, 2H), 6.68 (d, J = 7.9 Hz, 3H), 5.43 (d, J = 16.1 Hz, 1H), 4.96 (d, J = 16.0 Hz, 1H), 4.81 (d, J = 3.0 Hz, 1H), 4.68 (d, J = 2.9 Hz, 1H), 4.20 – 4.14 (m, 1H), 3.98 (t, J = 7.6 Hz, 1H), 3.87 (t, J = 8.8 Hz, 1H), 2.34 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.7, 145.8, 137.0, 134.5, 133.4, 129.7, 129.6, 129.6, 126.5, 124.2, 120.3, 117.6, 116.1, 112.3, 111.8, 64.8, 58.9, 48.5, 45.6, 21.2.

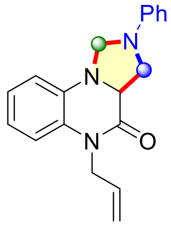
5-(4-methoxybenzyl)-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one(4fa)[2]



^1H NMR (500 MHz, $CDCl_3$) δ 7.32 (t, J = 7.8 Hz, 2H), 7.20 (d, J = 8.5 Hz, 2H), 7.05 (t, J = 7.6 Hz, 1H), 6.99 (d, J = 8.0 Hz, 1H), 6.89 – 6.80 (m, 4H), 6.67 (d, J = 8.0 Hz, 3H), 5.36 (d, J = 15.9 Hz, 1H), 4.97 (d, J = 15.9 Hz, 1H), 4.81 (d, J = 3.2 Hz, 1H), 4.68 (d, J = 3.2 Hz, 1H), 4.18 – 4.13 (m, 1H), 4.00 – 3.94 (m, 1H), 3.86 (t, J = 8.9 Hz, 1H), 3.78 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.8, 158.9, 145.8, 134.6, 129.7, 129.6, 128.5, 128.0, 124.2, 120.3, 117.6, 116.1, 114.3, 112.3, 111.8, 64.8, 59.0, 55.4, 48.6, 45.3.

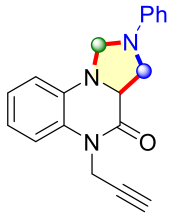
5-allyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one(4ga)[1]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 (t, J = 7.7 Hz, 2H), 7.12 – 7.03 (m, 2H), 6.94 (t, J = 7.7 Hz, 1H), 6.82 (t, J = 7.3 Hz, 1H), 6.70 – 6.62 (m, 3H), 5.97 – 5.88 (m, 1H), 5.28 – 5.21 (m, 2H), 4.89 – 4.82 (m, 1H), 4.78 (d, J = 3.2 Hz, 1H), 4.66 (d, J = 3.2 Hz, 1H), 4.43 – 4.35 (m, 1H), 4.10 – 4.04 (m, 1H), 3.92 (t, J = 7.6 Hz, 1H), 3.80 (t, J = 8.8 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.3, 145.8, 134.5, 132.1, 129.7, 129.5, 124.2, 120.3, 117.5, 117.0, 115.8, 112.3, 111.8, 64.7, 58.8, 48.4, 44.7.

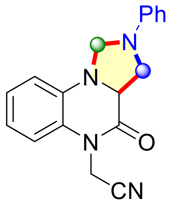
2-phenyl-5-(prop-2-yn-1-yl)-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one (4ha)[1]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 – 7.24 (m, 3H), 7.11 (t, J = 7.5 Hz, 1H), 7.00 (t, J = 7.6 Hz, 1H), 6.81 (t, J = 7.2 Hz, 1H), 6.68 (d, J = 7.7 Hz, 1H), 6.63 (d, J = 7.7 Hz, 2H), 5.02 (d, J = 17.6 Hz, 1H), 4.76 (s, 1H), 4.66 (s, 1H), 4.46 (d, J = 17.6 Hz, 1H), 4.06 (t, J = 7.8 Hz, 1H), 3.92 (t, J = 7.5 Hz, 1H), 3.77 (t, J = 8.8 Hz, 1H), 2.27 (s, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.1, 145.7, 134.4, 129.6, 128.9, 124.6, 120.4, 117.7, 115.7, 112.4, 111.8, 78.2, 72.4, 64.7, 58.9, 48.4, 31.7.

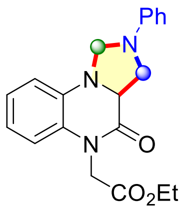
2-(4-oxo-2-phenyl-2,3,3a,4-tetrahydroimidazo[1,5-a]quinoxalin-5(1*H*)-yl)acetonitrile (4ia)[1]



^{1}H NMR (500 MHz, DMSO-d_6) δ 7.30 (d, *J* = 7.4 Hz, 1H), 7.24 (s, 2H), 7.15 (s, 1H), 7.03 (d, *J* = 6.9 Hz, 1H), 6.92 (d, *J* = 7.0 Hz, 1H), 6.77 – 6.66 (m, 3H), 5.23 – 5.10 (m, 2H), 4.82 (s, 1H), 4.54 (s, 1H), 4.29 – 4.18 (m, 1H), 3.84 (s, 1H), 3.59 (t, *J* = 8.1 Hz, 1H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 165.2, 145.7, 134.5, 129.2, 127.7, 124.7, 120.1, 116.9, 116.3, 115.2, 113.2, 111.9, 64.5, 58.0, 47.7, 29.8.

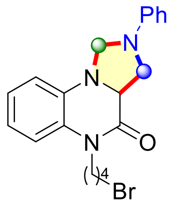
Ethyl-2-(4-oxo-2-phenyl-2,3,3a,4-tetrahydroimidazo[1,5-a]quinoxalin-5(1*H*)-yl)acetate(4ja)[1]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 (t, *J* = 7.8 Hz, 2H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.94 (t, *J* = 7.6 Hz, 1H), 6.81 (t, *J* = 8.7 Hz, 2H), 6.69 (d, *J* = 7.8 Hz, 1H), 6.64 (d, *J* = 8.1 Hz, 2H), 5.04 (d, *J* = 17.6 Hz, 1H), 4.78 (d, *J* = 3.2 Hz, 1H), 4.66 (d, *J* = 3.1 Hz, 1H), 4.38 (d, *J* = 17.6 Hz, 1H), 4.29 – 4.24 (m, 2H), 4.14 – 4.09 (m, 1H), 3.92 (t, *J* = 7.7 Hz, 1H), 3.78 (t, *J* = 8.8 Hz, 1H), 1.30 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 168.3, 165.9, 145.7, 134.3, 129.5, 124.4, 120.4, 117.6, 114.7, 112.6, 111.8, 64.7, 61.8, 58.7, 48.3, 44.0, 14.2.

5-(4-bromobutyl)-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4ka）

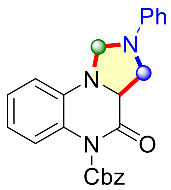


^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 (t, J = 7.8 Hz, 2H), 7.19 (d, J = 8.0 Hz, 1H), 7.09 (t, J = 7.6 Hz, 1H), 6.97 (t, J = 7.7 Hz, 1H), 6.81 (t, J = 7.3 Hz, 1H), 6.70 – 6.61 (m, 3H), 4.79 (d, J = 3.2 Hz, 1H), 4.66 (d, J = 3.1 Hz, 1H), 4.08 – 4.03 (m, 1H), 4.02 – 3.96 (m, 1H), 3.94 – 3.89 (m, 1H), 3.89 – 3.83 (m, 1H), 3.78 (t, J = 8.8 Hz, 1H), 1.65 (s, 1H), 1.24 – 1.16 (m, 1H), 0.58 – 0.47 (m, 3H), 0.46 – 0.39 (m, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.4, 145.8, 134.6, 129.7, 129.6, 124.0, 120.2, 117.5, 115.6, 112.4, 111.8, 64.8, 58.8, 48.6, 46.0, 9.9, 4.5, 4.0.

HRMS (ESI) m/z calcd for $C_{20}H_{23}BrN_3O$ $[M+H]^+$:   400.1019, Found:400.1023

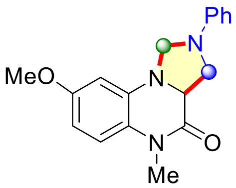
Benzyl-4-oxo-2-phenyl-2,3,3a,4-tetrahydroimidazo[1,5-a]quinoxaline-5(1*H*)-carboxylate (4la)[3]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 – 7.28 (m, 4H), 7.25 (d, J = 7.2 Hz, 3H), 7.03 (t, J = 7.6 Hz, 1H), 6.93 (d, J = 8.0 Hz, 1H), 6.81 (t, J = 7.7 Hz, 2H), 6.65 (d, J = 7.8 Hz, 3H), 5.44 (d, J = 16.2 Hz, 1H), 4.97 (d, J = 16.2 Hz, 1H), 4.79 (d, J = 3.2 Hz, 1H), 4.66 (d, J = 3.2 Hz, 1H), 4.15 (d, J = 7.4 Hz, 1H), 3.95 (t, J = 7.7 Hz, 1H), 3.84 (t, J = 8.9 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.8, 145.8, 136.5, 134.6, 129.7, 129.6, 128.9, 127.4, 126.6, 124.2, 120.3, 117.6, 116.1, 112.3, 111.8, 64.8, 58.9, 48.6, 45.9.

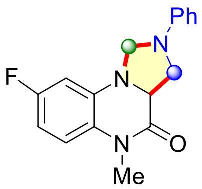
8-methoxy-5-methyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one (4ma)[2]



[1]H NMR (500 MHz, $CDCl_3$) δ 7.30 (t, *J* = 7.9 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 1H), 6.81 (t, *J* = 7.3 Hz, 1H), 6.63 (d, *J* = 8.1 Hz, 2H), 6.51 – 6.42 (m, 1H), 6.22 (d, *J* = 2.6 Hz, 1H), 4.73 (d, *J* = 3.4 Hz, 1H), 4.62 (d, *J* = 3.3 Hz, 1H), 4.06 – 4.01 (m, 1H), 3.94 – 3.90 (m, 1H), 3.82 (s, 3H), 3.73 (t, *J* = 8.9 Hz, 1H), 3.39 (s, 3H).

[13]C NMR (126 MHz, $CDCl_3$) δ 164.9, 156.7, 145.8, 135.4, 129.6, 124.3, 117.6, 115.8, 111.8, 103.6, 99.4, 64.7, 58.8, 55.7, 48.6, 29.2.

8-fluoro-5-methyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one (4na)[1]

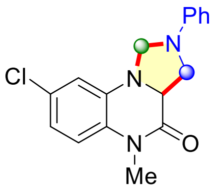


[1]H NMR (500 MHz, $CDCl_3$) δ 7.31 (t, *J* = 7.8 Hz, 2H), 6.95 – 6.89 (m, 1H), 6.82 (t, *J* = 7.3 Hz, 1H), 6.67 – 6.59 (m, 3H), 6.41 – 6.34 (m, 1H), 4.70 (d, *J* = 3.3 Hz, 1H), 4.63 (d, *J* = 3.3 Hz, 1H), 4.10 – 4.05 (m, 1H), 3.97 – 3.90 (m, 1H), 3.72 (t, *J* = 8.9 Hz, 1H), 3.40 (s, 3H).

[13]C NMR (126 MHz, $CDCl_3$) δ 164.8,159 (d, *J* =121.6 Hz), 154.6, 135.4(d, *J* =5.6 Hz), 129.6, 126.5(d, *J* =2.5 Hz) 117.8, 115.9 (d, *J* =5.0 Hz) , 111.9,105.7 (d, *J* =11.9 Hz) , 99.8 (d, *J* =13.2 Hz) , 64.6, 58.4, 48.7, 29.2.

[19]F NMR (471 MHz, $CDCl_3$) δ -118.2.

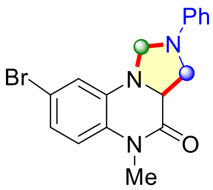
8-chloro-5-methyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one (4oa)[3]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (t, J = 7.9 Hz, 2H), 6.90 (s, 2H), 6.82 (t, J = 7.3 Hz, 1H), 6.65 – 6.60 (m, 3H), 4.70 (d, J = 3.3 Hz, 1H), 4.65 (d, J = 3.3 Hz, 1H), 4.10 – 4.05 (m, 1H), 3.96 – 3.91 (m, 1H), 3.71 (t, J = 8.9 Hz, 1H), 3.39 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.0, 145.6, 135.0, 129.6, 129.4, 129.0, 119.6, 117.8, 115.9, 112.1, 111.9, 64.6, 58.5, 48.6, 29.2.

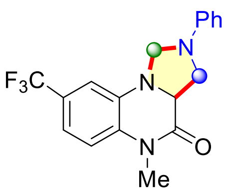
8-bromo-5-methyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one (4pa)[3]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (t, J = 7.9 Hz, 2H), 7.07 – 7.02 (m, 1H), 6.86 – 6.80 (m, 2H), 6.74 (d, J = 1.9 Hz, 1H), 6.62 (d, J = 8.2 Hz, 2H), 4.69 (d, J = 3.4 Hz, 1H), 4.63 (d, J = 3.4 Hz, 1H), 4.09 – 4.04 (m, 1H), 3.95 – 3.90 (m, 1H), 3.71 (t, J = 8.9 Hz, 1H), 3.38 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.0, 145.6, 135.2, 129.6, 129.4, 122.6, 117.8, 116.9, 116.3, 114.8, 111.9, 64.6, 58.4, 48.6, 29.1.

5-methyl-2-phenyl-8-(trifluoromethyl)-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one(4pa)[5]



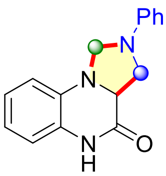
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 (t, J = 7.7 Hz, 2H), 7.22 (d, J = 8.2 Hz, 1H), 7.07 (d, J = 8.3 Hz, 1H), 6.84 (d, J = 7.8 Hz, 2H), 6.65 (d, J = 8.0 Hz, 2H), 4.76 (d, J = 2.8

Hz, 1H), 4.72 (s, 1H), 4.15 – 4.09 (m, 1H), 3.95 (t, *J* = 7.6 Hz, 1H), 3.74 (t, *J* = 8.8 Hz, 1H), 3.44 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.3, 145.6, 134.2, 132.9, 129.6, 126.2(q, *J* =65.5 Hz) 124.2(q, *J* = 544.3Hz), 117.9,117.6 (q, *J* = 8.8 Hz) , 114.9, 112.0,108.6 (q, *J* =7.6 Hz), 64.6, 58.4, 48.6, 29.2.

^{19}F NMR (471 MHz, $CDCl_3$) δ -62.0.

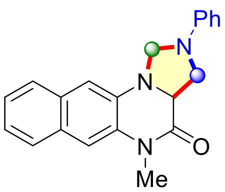
2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one (4ra)[2]



^{1}H NMR (500 MHz, DMSO-d_6) δ 10.61 (s, 1H), 7.23 (t, *J* = 7.4 Hz, 2H), 6.99 – 6.90 (m, 2H), 6.84 – 6.77 (m, 2H), 6.74 – 6.65 (m, 3H), 4.79 (d, *J* = 3.8 Hz, 1H), 4.52 (d, *J* = 3.8 Hz, 1H), 4.11 (t, *J* = 7.8 Hz, 1H), 3.76 (t, *J* = 7.6 Hz, 1H), 3.50 (t, *J* = 8.7 Hz, 1H).

^{13}C NMR (126 MHz, DMSO-d_6) δ 165.7, 145.9, 132.8, 129.2, 127.9, 123.2, 119.7, 116.8, 115.2, 112.6, 111.9, 64.6, 58.0, 47.8.

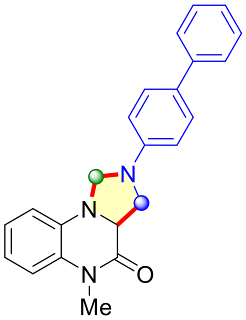
5-methyl-2-phenyl-1,2,3,3a-tetrahydrobenzo[g]imidazo[1,5-a]quinoxalin-4(5*H*)-one (4sa)[2]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 – 7.68 (m, 2H), 7.41 (t, *J* = 7.4 Hz, 1H), 7.36 – 7.29 (m, 4H), 6.87 – 6.82 (m, 2H), 6.66 (d, *J* = 8.1 Hz, 2H), 4.78 (d, *J* = 3.4 Hz, 1H), 4.67 (d, *J* = 3.3 Hz, 1H), 4.09 – 4.04 (m, 1H), 3.94 (t, *J* = 7.6 Hz, 1H), 3.73 (t, *J* = 8.9 Hz, 1H), 3.50 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 166.1, 145.7, 133.7, 131.3, 130.9, 129.5, 128.5, 127.5, 125.9, 124.1, 117.6, 112.3, 111.8, 107.0, 64.8, 58.7, 48.6, 29.3.

2-([1,1'-biphenyl]-4-yl)-5-methyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4ab）

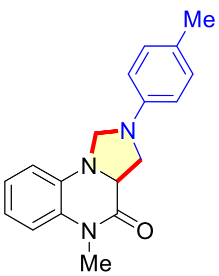


^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (t, J = 7.4 Hz, 4H), 7.29 (t, J = 7.5 Hz, 2H), 7.16 (t, J = 7.2 Hz, 1H), 6.97 (t, J = 7.5 Hz, 1H), 6.90 (d, J = 7.8 Hz, 1H), 6.85 (t, J = 7.6 Hz, 1H), 6.57 (d, J = 8.3 Hz, 2H), 6.53 (d, J = 7.7 Hz, 1H), 4.65 (d, J = 2.9 Hz, 1H), 4.53 (d, J = 2.9 Hz, 1H), 3.92 – 3.86 (m, 1H), 3.82 (t, J = 7.5 Hz, 1H), 3.66 (t, J = 8.7 Hz, 1H), 3.28 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.5, 145.1, 141.0, 134.2, 130.4, 130.3, 128.8, 128.1, 126.4, 126.3, 124.1, 120.3, 115.2, 112.1, 112.1, 64.6, 58.8, 48.6, 29.1.

HRMS (ESI) m/z calcd for $C_{23}H_{22}N_3O$ $[M+H]^+$: 356.1757, found: 356.1753

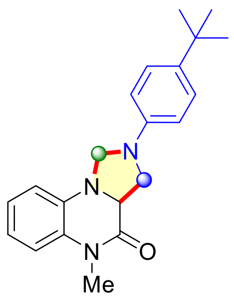
5-methyl-2-(p-tolyl)-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one (4ac)[4]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.12 (d, J = 8.2 Hz, 2H), 7.08 (t, J = 8.0 Hz, 1H), 7.03 (d, J = 7.7 Hz, 1H), 6.96 (t, J = 7.7 Hz, 1H), 6.66 (d, J = 7.7 Hz, 1H), 6.57 (d, J = 8.3 Hz, 2H), 4.72 (d, J = 3.2 Hz, 1H), 4.65 (d, J = 3.2 Hz, 1H), 4.07 – 4.01 (m, 1H), 3.93 – 3.88 (m, 1H), 3.73 (t, J = 8.8 Hz, 1H), 3.42 (s, 3H), 2.29 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.6, 143.8, 134.3, 130.4, 130.0, 126.8, 124.1, 120.1, 115.1, 112.1, 111.9, 65.0, 58.8, 48.8, 29.1, 20.4.

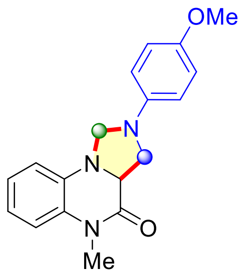
2-(4-(tert-butyl)phenyl)-5-methyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one (4ad)[3]



[1]H NMR (500 MHz, $CDCl_3$) δ 7.35 (d, *J* = 8.5 Hz, 2H), 7.09 (t, *J* = 7.6 Hz, 1H), 7.03 (d, *J* = 7.8 Hz, 1H), 6.96 (d, *J* = 7.6 Hz, 1H), 6.67 (d, *J* = 7.7 Hz, 1H), 6.61 (d, *J* = 8.6 Hz, 2H), 4.76 (d, *J* = 3.1 Hz, 1H), 4.67 (d, *J* = 3.1 Hz, 1H), 4.07 – 4.02 (m, 1H), 3.96 – 3.90 (m, 1H), 3.75 (t, *J* = 8.8 Hz, 1H), 3.43 (s, 3H), 1.32 (s, 9H).

[13]C NMR (126 MHz, $CDCl_3$) δ 165.7, 143.7, 140.3, 134.4, 130.5, 126.4, 124.1, 120.2, 115.2, 112.2, 111.6, 64.9, 58.9, 48.8, 34.0, 31.7, 29.1.

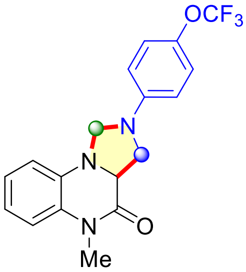
2-(4-methoxyphenyl)-5-methyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one (4ae)[1]



[1]H NMR (500 MHz, $CDCl_3$) δ 7.07 (t, *J* = 7.6 Hz, 1H), 7.02 (d, *J* = 7.9 Hz, 1H), 6.95 (t, *J* = 8.3 Hz, 1H), 6.90 (d, *J* = 8.8 Hz, 2H), 6.65 (d, *J* = 7.7 Hz, 1H), 6.60 (d, *J* = 8.8 Hz, 2H), 4.67 (d, *J* = 5.6 Hz, 2H), 4.09 – 4.04 (m, 1H), 3.87 (t, *J* = 7.5 Hz, 1H), 3.78 (s, 3H), 3.70 (t, *J* = 8.7 Hz, 1H), 3.41 (s, 3H).

[13]C NMR (126 MHz, $CDCl_3$) δ 165.6, 152.2, 140.7, 134.3, 130.4, 124.1, 120.1, 115.2, 115.1, 112.9, 112.2, 65.5, 58.9, 55.9, 49.3, 29.1.

5-methyl-2-(4-(trifluoromethoxy)phenyl)-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one (4af)[5]

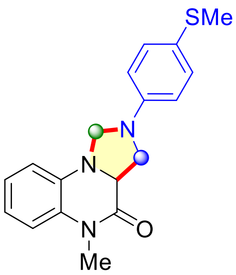


^{1}H NMR (500 MHz, $CDCl_3$) δ 7.16 (d, J = 8.6 Hz, 2H), 7.11 – 7.06 (m, 1H), 7.06 – 7.02 (m, 1H), 7.01 – 6.96 (m, 1H), 6.67 – 6.64 (m, 1H), 6.57 (d, J = 9.0 Hz, 2H), 4.74 (d, J = 3.3 Hz, 1H), 4.63 (d, J = 3.3 Hz, 1H), 4.07 – 4.02 (m, 1H), 3.92 – 3.86 (m, 1H), 3.75 (t, J = 8.8 Hz, 1H), 3.42 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.4, 144.6, 140.7, 134.1, 130.5, 124.2, 122.8, 120.8(d, J = 127.9Hz), 120.5, 115.3, 112.2, 112.1, 64.8, 58.9, 48.8, 29.1.

^{19}F NMR (471 MHz, $CDCl_3$) δ -58.5.

5-methyl-2-(4-(methylthio)phenyl)-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4ag）

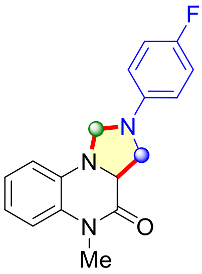


^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 (d, J = 8.0 Hz, 2H), 7.08 (t, J = 7.5 Hz, 1H), 7.03 (d, J = 7.9 Hz, 1H), 6.96 (t, J = 7.6 Hz, 1H), 6.64 (d, J = 7.7 Hz, 1H), 6.57 (d, J = 8.1 Hz, 2H), 4.73 (s, 1H), 4.62 (s, 1H), 4.02 (t, J = 7.9 Hz, 1H), 3.89 (t, J = 7.6 Hz, 1H), 3.74 (d, J = 8.8 Hz, 1H), 3.41 (s, 3H), 2.43 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.5, 144.5, 134.2, 131.5, 130.4, 124.8, 124.1, 120.3, 115.2, 112.5, 112.2, 64.7, 58.8, 48.6, 29.1, 19.1.

HRMS (ESI) m/z calcd for $C_{18}H_{20}N_3OS$ $[M+H]^+$: 326.1322, found 326.1325

2-(4-fluorophenyl)-5-methyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one (4ah)[1]

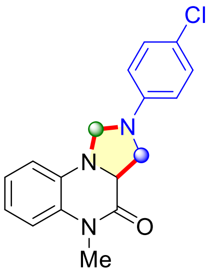


^{1}H NMR (500 MHz, $CDCl_3$) δ 7.08 (t, J = 7.5 Hz, 1H), 7.05 – 6.94 (m, 4H), 6.64 (d, J = 7.7 Hz, 1H), 6.57 – 6.52 (m, 2H), 4.70 (s, 1H), 4.65 (s, 1H), 4.05 (t, J = 7.8 Hz, 1H), 3.87 (t, J = 7.5 Hz, 1H), 3.72 (t, J = 8.7 Hz, 1H), 3.42 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.5,156.0 (d, J = 118.44 Hz), 142.5, 134.2, 130.4, 124.1, 120.3, 116.05(d, J = 22.68Hz), 115.2, 112.5(d, J = 7.6 Hz), 112.2, 65.3, 58.9, 49.1, 29.1.

^{19}F NMR (471 MHz, $CDCl_3$) δ -128.0.

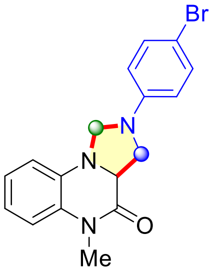
2-(4-chlorophenyl)-5-methyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one (4ai)[1]



^{13}C NMR (126 MHz, $CDCl_3$) δ 7.23 (d, J = 8.8 Hz, 2H), 7.08 (t, J = 7.3 Hz, 1H), 7.03 (d, J = 7.5 Hz, 1H), 6.97 (t, J = 7.6 Hz, 1H), 6.64 (d, J = 7.7 Hz, 1H), 6.53 (d, J = 8.8 Hz, 2H), 4.71 (d, J = 3.3 Hz, 1H), 4.61 (d, J = 3.3 Hz, 1H), 4.06 – 4.01 (m, 1H), 3.89 – 3.84 (m, 1H), 3.72 (t, J = 8.8 Hz, 1H), 3.41 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.4, 144.4, 134.1, 130.5, 129.4, 124.2, 122.5, 120.4, 115.3, 112.9, 112.2, 64.8, 58.8, 48.7, 29.1.

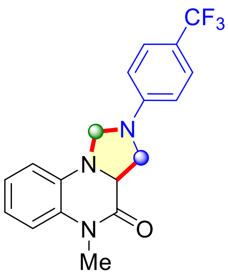
2-(4-bromophenyl)-5-methyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one (4aj)[2]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 (d, *J* = 8.8 Hz, 2H), 7.08 (t, *J* = 7.5 Hz, 1H), 7.02 (d, *J* = 7.7 Hz, 1H), 6.97 (t, *J* = 7.6 Hz, 1H), 6.63 (d, *J* = 7.8 Hz, 1H), 6.47 (d, *J* = 8.7 Hz, 2H), 4.69 (d, *J* = 3.3 Hz, 1H), 4.58 (d, *J* = 3.3 Hz, 1H), 4.04 – 3.99 (m, 1H), 3.87 – 3.83 (m, 1H), 3.70 (t, *J* = 8.8 Hz, 1H), 3.40 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.4, 144.7, 134.1, 132.2, 130.4, 124.1, 120.4, 115.2, 113.3, 112.2, 109.5, 64.6, 58.8, 48.6, 29.1.

5-methyl-2-(4-(trifluoromethyl)phenyl)-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one (4ak)[2]

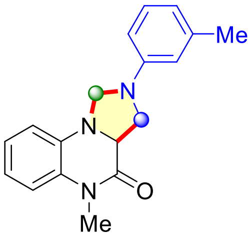


^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.5 Hz, 2H), 7.10 (t, *J* = 7.5 Hz, 1H), 7.05 (d, *J* = 7.7 Hz, 1H), 7.00 (t, *J* = 7.6 Hz, 1H), 6.69 – 6.62 (m, 3H), 4.83 (d, *J* = 3.4 Hz, 1H), 4.66 (d, *J* = 3.4 Hz, 1H), 4.08 – 4.03 (m, 1H), 3.98 – 3.94 (m, 1H), 3.81 (t, *J* = 8.9 Hz, 1H), 3.43 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.4, 147.8, 134.0, 130.6, 126.9 (q, *J* = 7.6 Hz), 125.1(d, *J* = 270.9 Hz), 124.2, 120.7, 119.2 (d, *J* =32.8 Hz), 115.4, 112.3, 111.2, 64.4, 58.8, 48.5, 29.2.

^{19}F NMR (471 MHz, $CDCl_3$) δ -61.0.

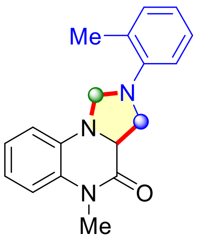
5-methyl-2-(m-tolyl)-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one(4al) [5]



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19 (t, J = 7.9 Hz, 1H), 7.09 (t, J = 7.5 Hz, 1H), 7.04 (d, J = 7.9 Hz, 1H), 6.97 (t, J = 7.5 Hz, 1H), 6.67 (d, J = 7.7 Hz, 1H), 6.64 (d, J = 7.4 Hz, 1H), 6.46 (d, J = 6.7 Hz, 2H), 4.76 (d, J = 2.8 Hz, 1H), 4.65 (d, J = 2.6 Hz, 1H), 4.06 – 4.01 (m, 1H), 3.92 (t, J = 7.6 Hz, 1H), 3.75 (t, J = 8.8 Hz, 1H), 3.43 (s, 3H), 2.36 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 165.7, 145.9, 139.4, 134.4, 130.5, 129.4, 124.1, 120.2, 118.5, 115.2, 112.6, 112.1, 109.1, 64.8, 58.8, 48.6, 29.1, 21.9.

5-methyl-2-(o-tolyl)-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5H)-one（4am）[5]



1H NMR (500 MHz, CDCl3) δ 7.07 – 7.00 (m, 2H), 6.91 (t, J = 7.6 Hz, 1H), 6.88 – 6.77 (m, 4H), 6.47 (d, J = 7.8 Hz, 1H), 4.65 (d, J = 4.7 Hz, 1H), 4.36 (d, J = 4.7 Hz, 1H), 3.94 – 3.89 (m, 1H), 3.71 (t, J = 9.1 Hz, 1H), 3.61 – 3.55 (m, 1H), 3.25 (s, 3H), 2.26 (s, 3H).

13C NMR (126 MHz, CDCl3) δ 165.4, 147.5, 134.2, 131.7, 130.1, 130.1, 126.6, 123.9, 122.4, 119.8, 117.0, 114.9, 112.9, 69.0, 58.1, 52.9, 28.8, 19.9.

4. Reference

1. Y.-F. Si, K. Sun, X.-L. Chen, X.-Y. Fu, Y. Liu, F.-L. Zeng, T. Shi, L.-B. Qu and B. Yu, *Org. Lett.*, 2020, **22**, 6960-6965.

2. J.-F. Cui, W.-Q. Zhong and J.-M. Huang, *J. Org. Chem.*, 2023, **88**, 1147-1154.

3. Z. Tang, C. Pi, Y. Wu and X. Cui, *Green Synth. Catal.*, 2022, DOI: 10.1016/j.gresc.2022.10.001.

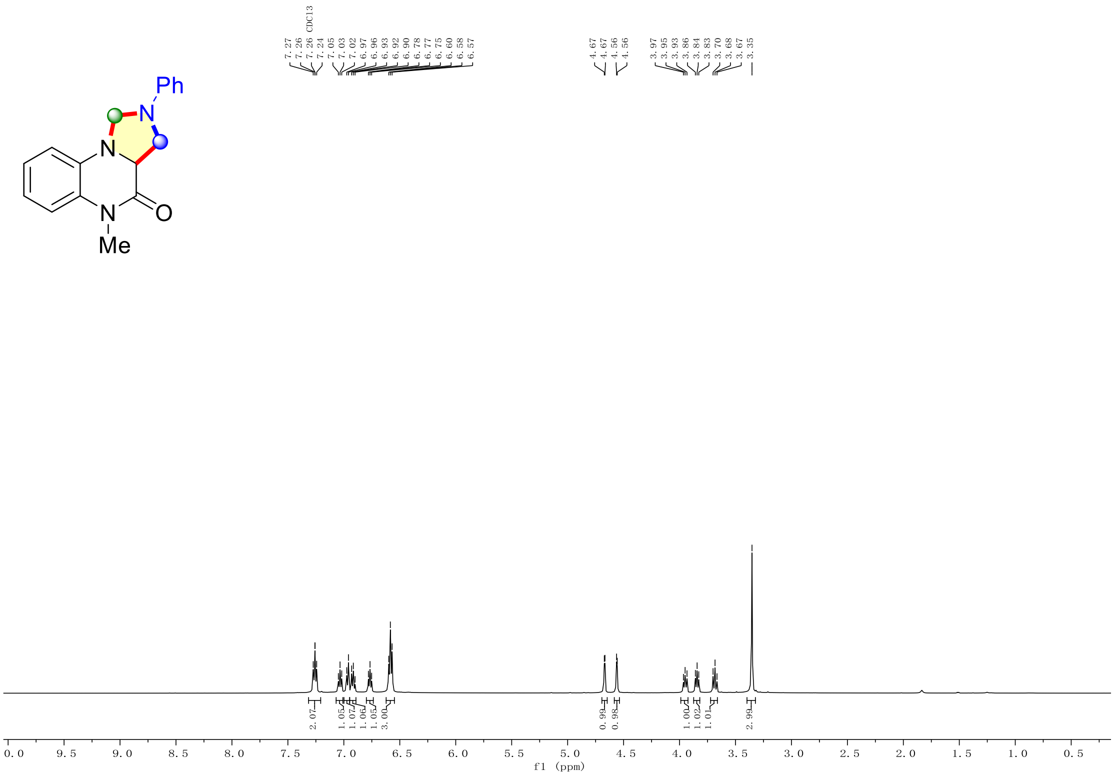
4. Y.-F. Si, X.-L. Chen, X.-Y. Fu, K. Sun, X. Song, L.-B. Qu and B. Yu, *ACS Sustainable Chem. Eng.*, 2020, **8**, 10740-10746.

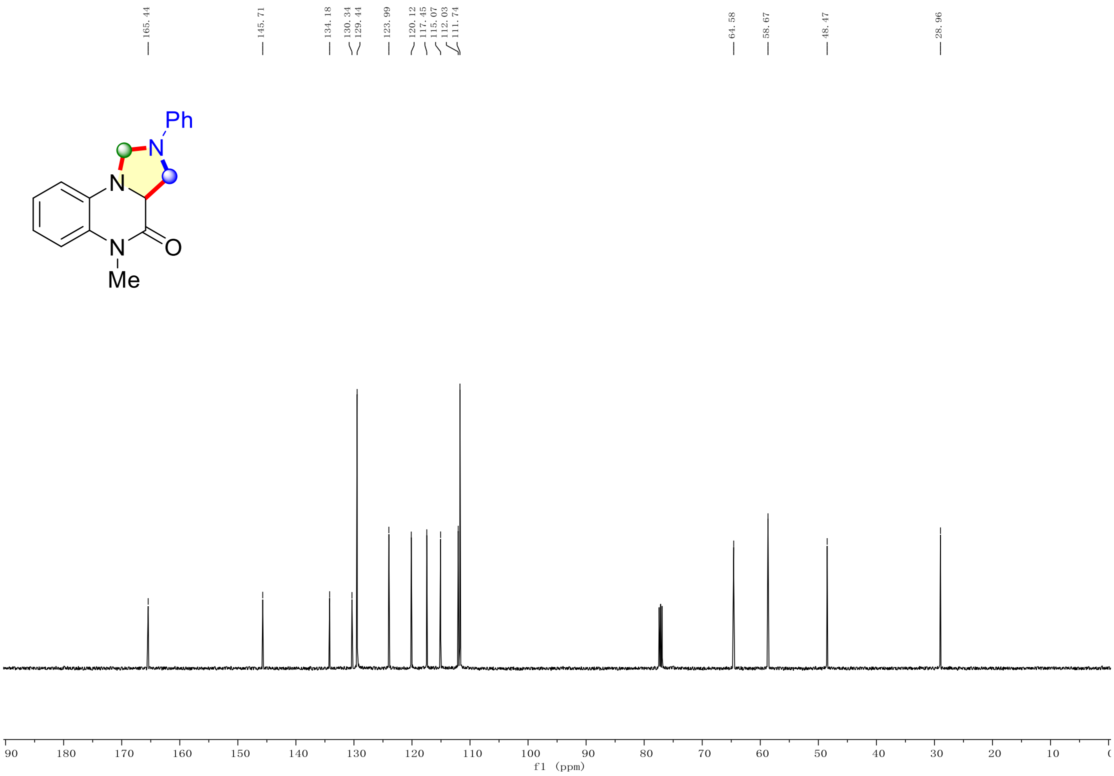
5. Y.-H. Lu, Z.-T. Zhang, H.-Y. Wu, M.-H. Zhou, H.-Y. Song, H.-T. Ji, J. Jiang, J.-Y. Chen and W.-M. He, *Chin. Chem. Lett.*, 2023, **34**, 108036.

5. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR Spectra of Products

5-methyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one (4aa)

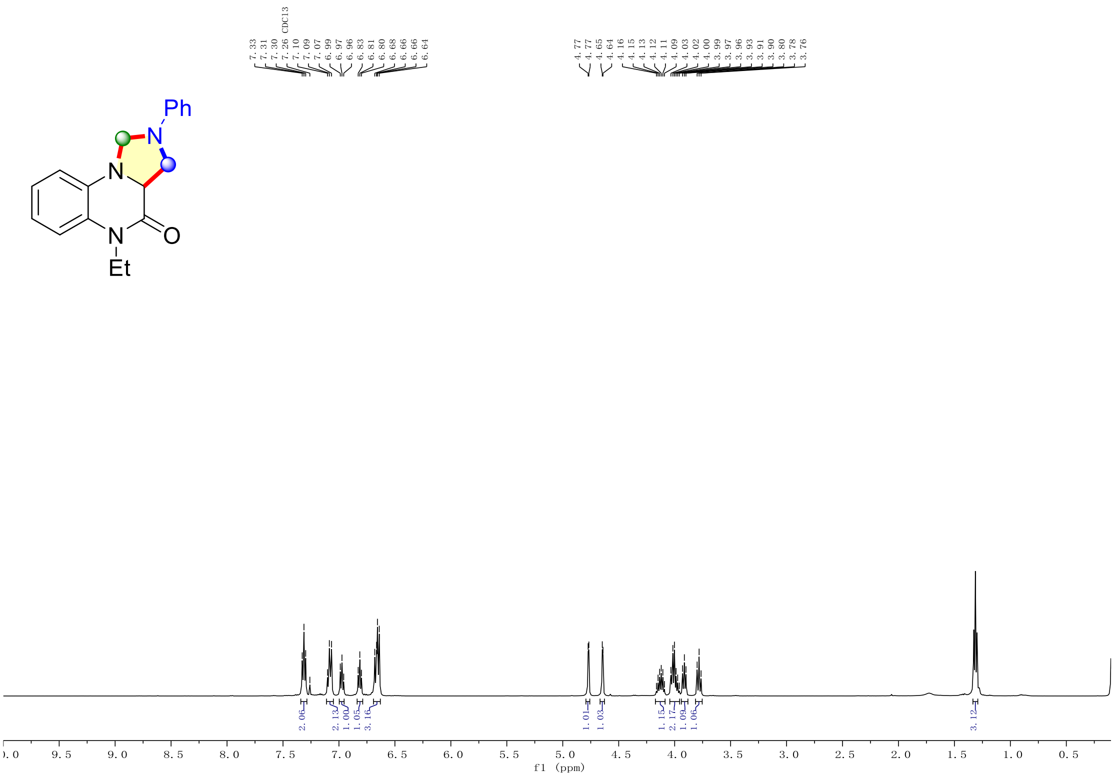
4aa ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

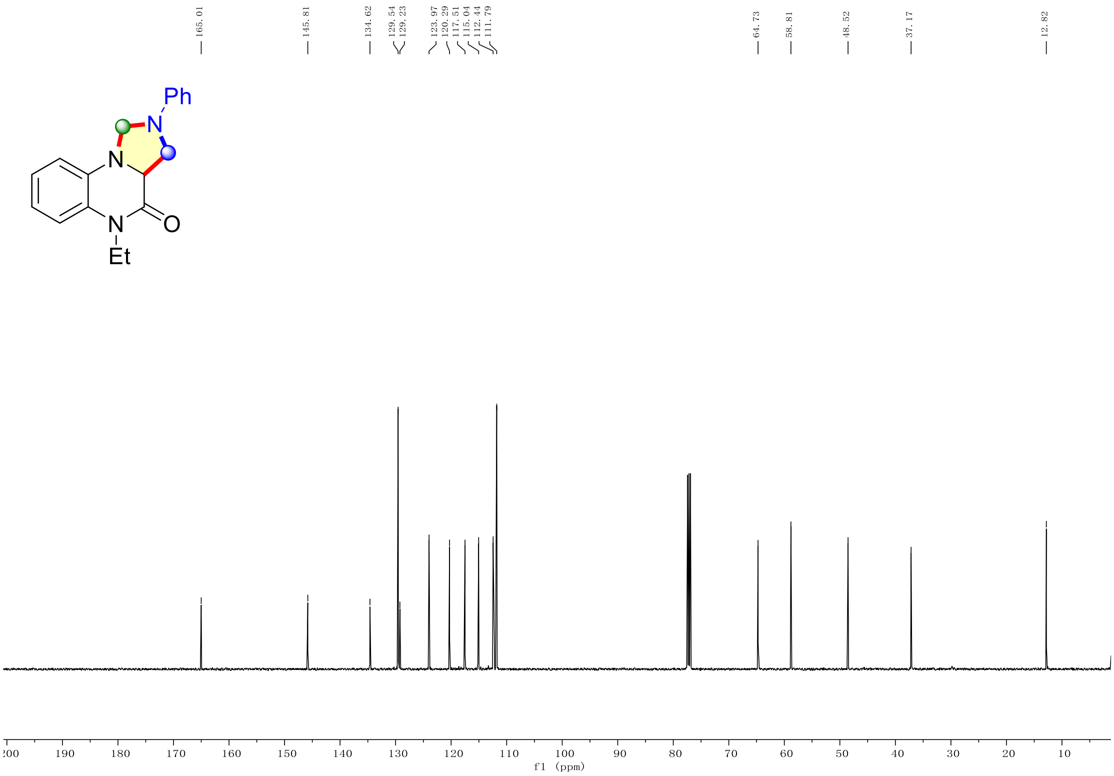




5-ethyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one(4ba)

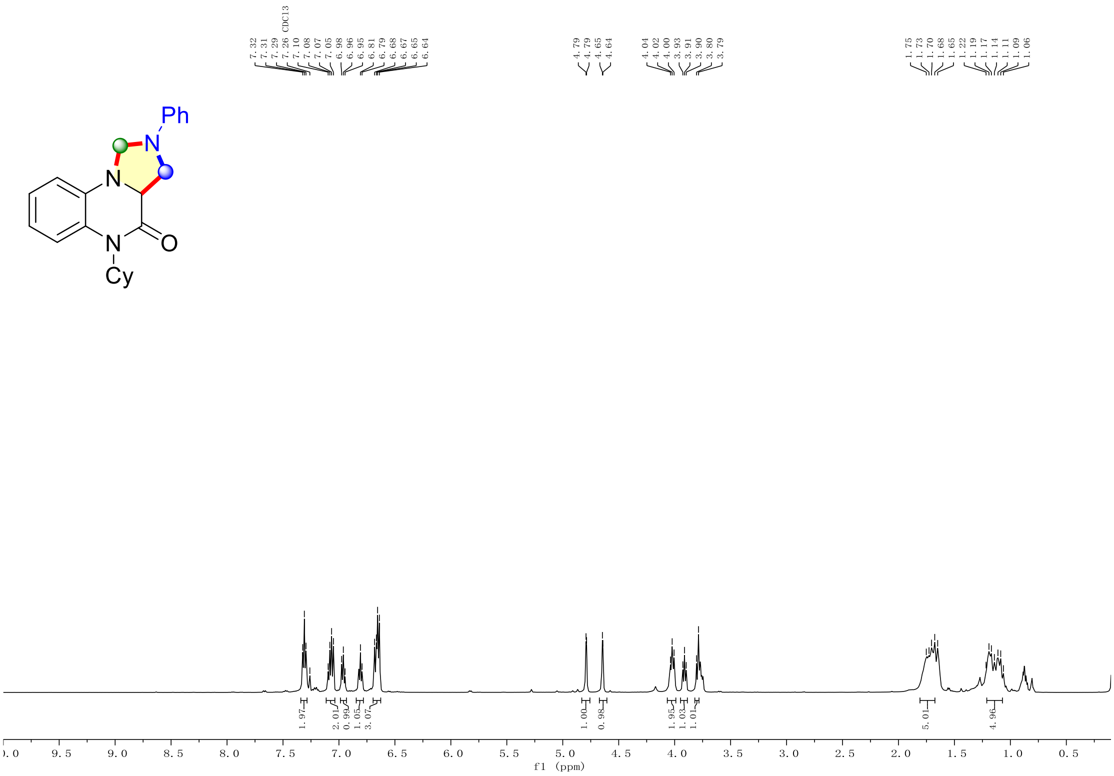
4ba ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

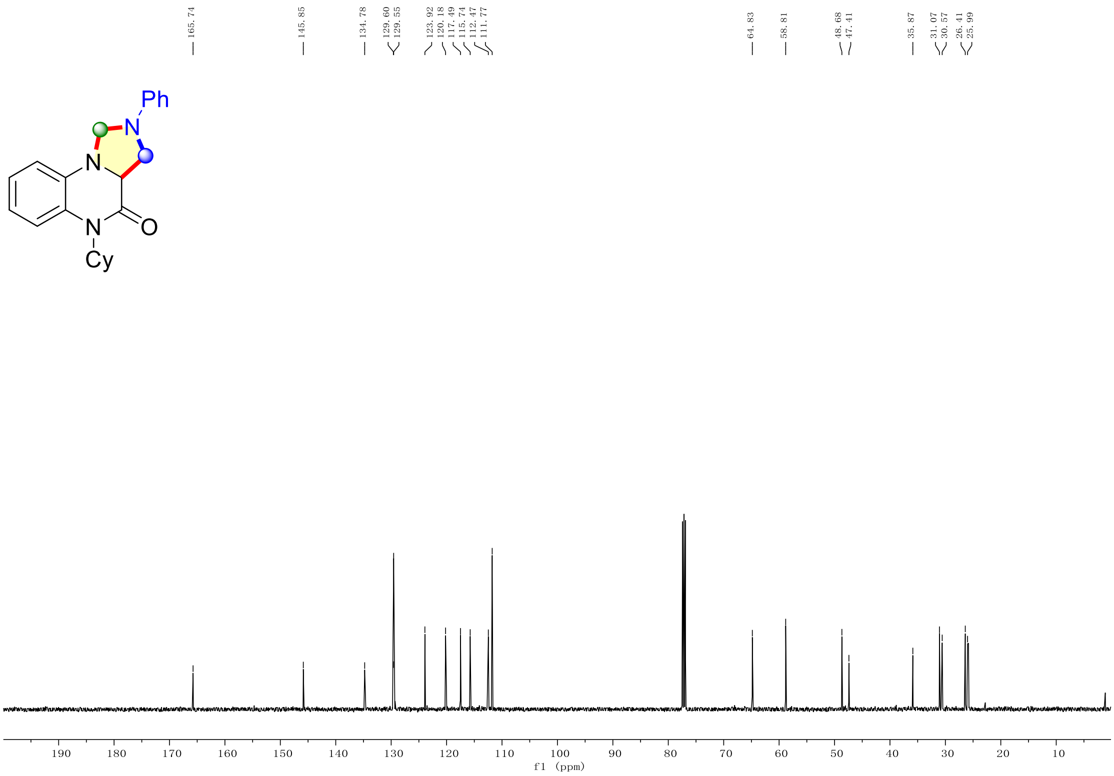




5-cyclohexyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one （4ca）

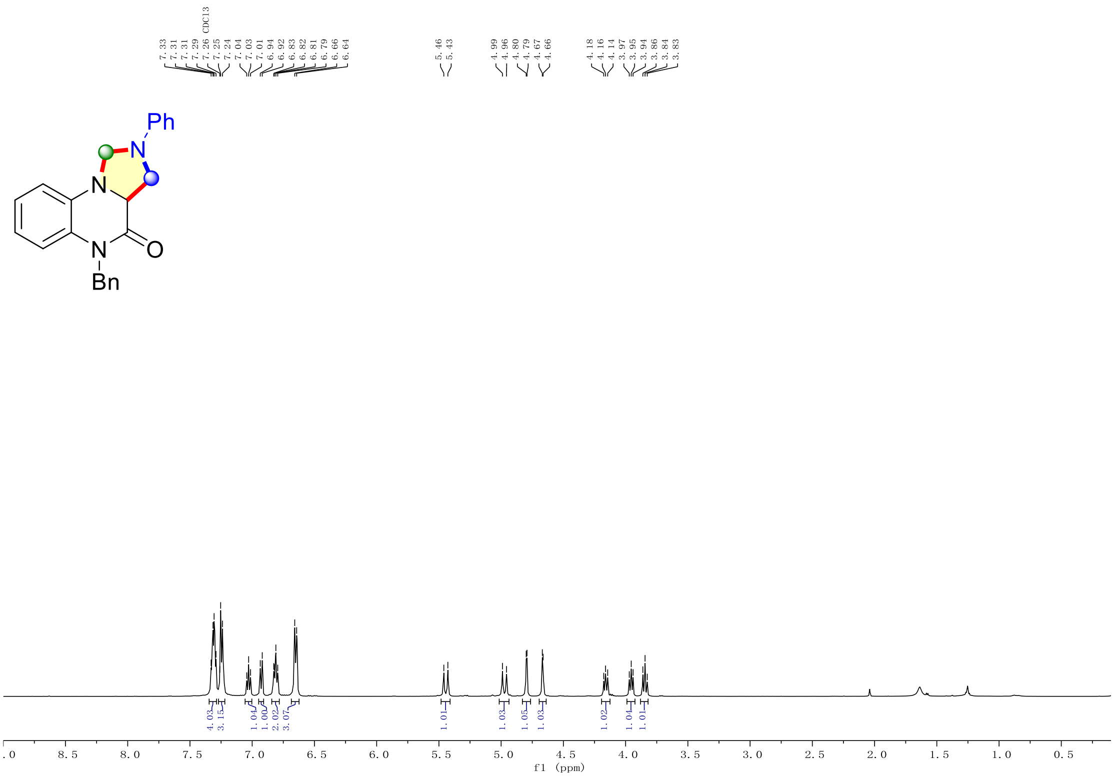
4ca ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

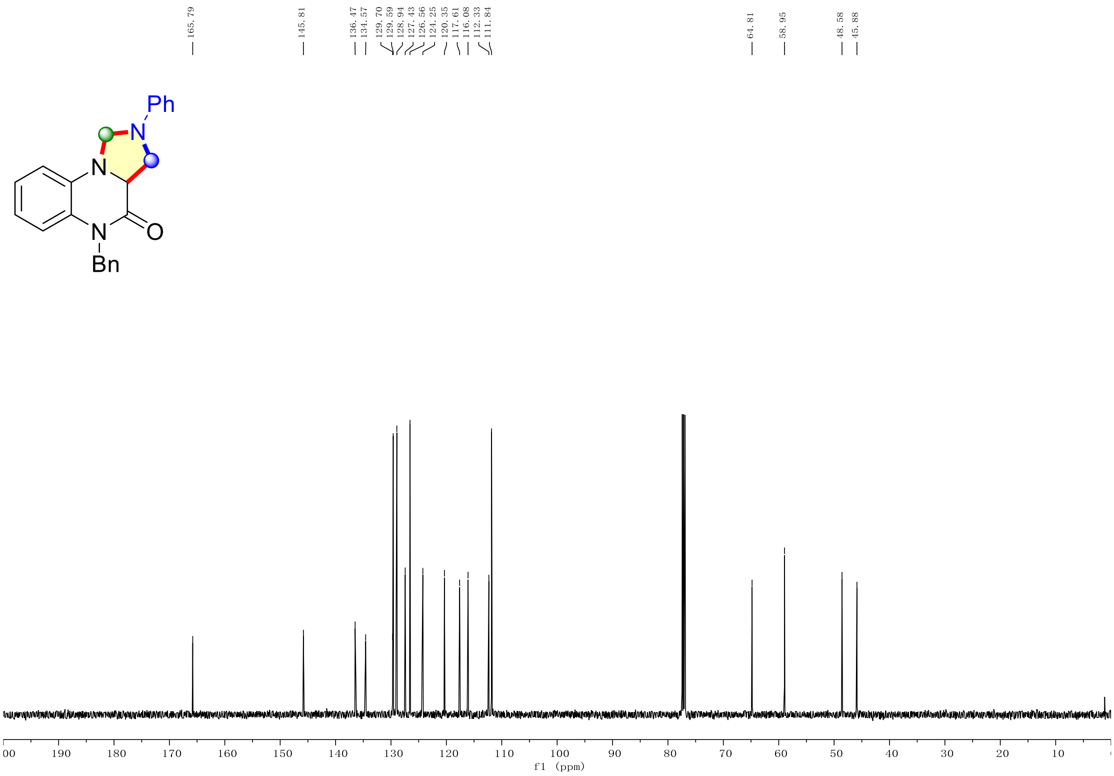




5-benzyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one(4da)

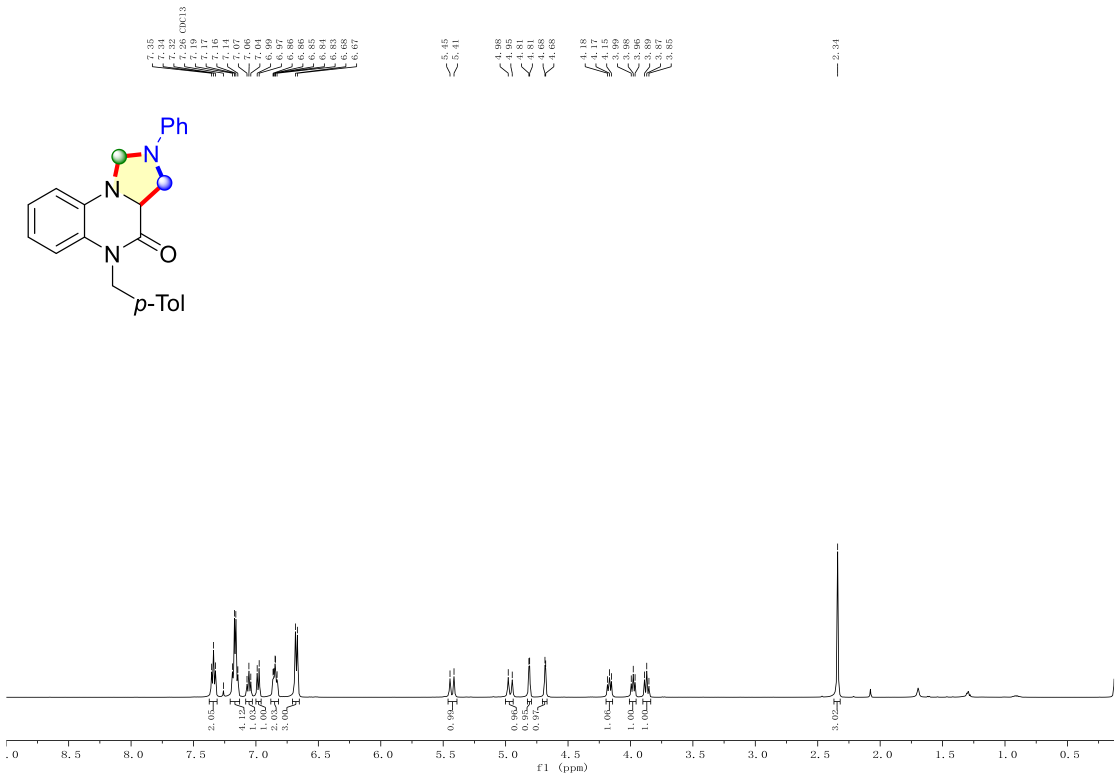
4da ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

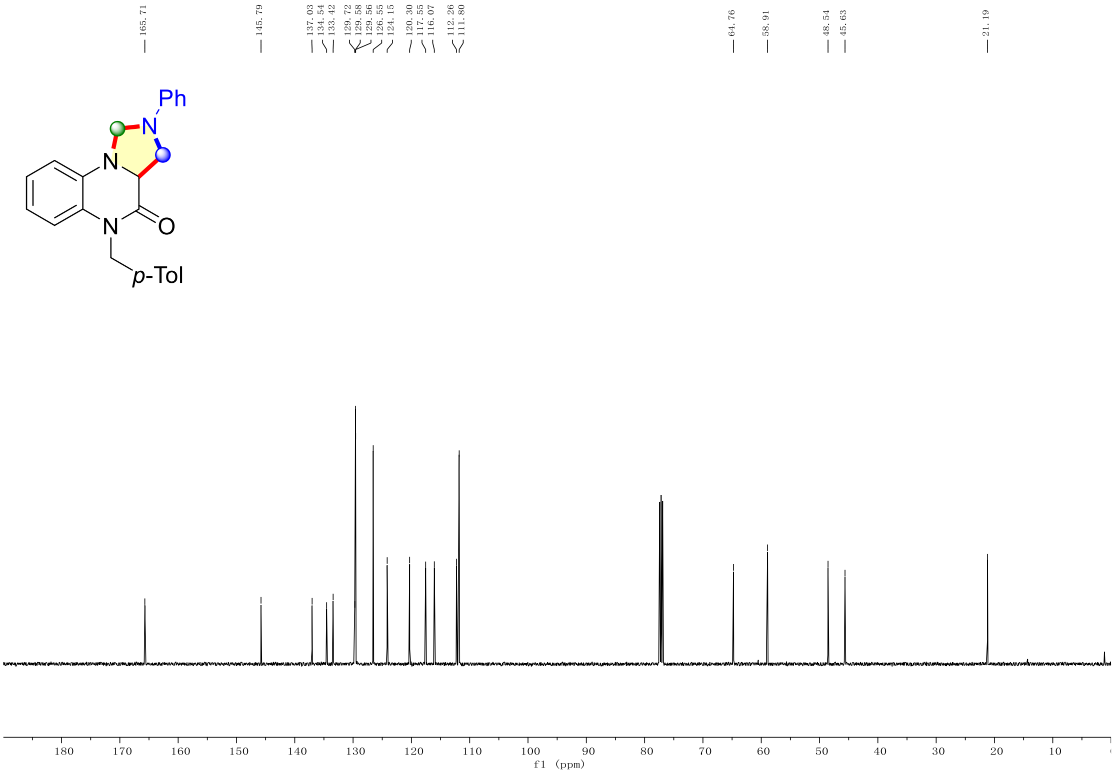




5-(4-methylbenzyl)-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4ea）

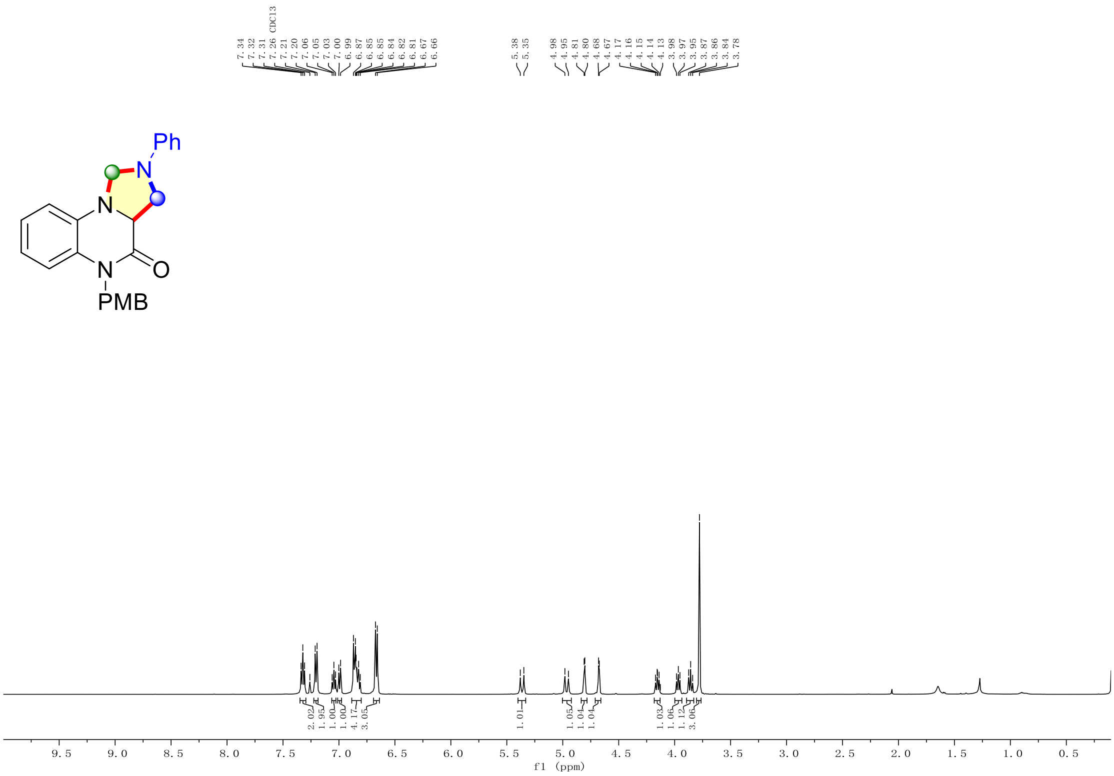
4ea ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

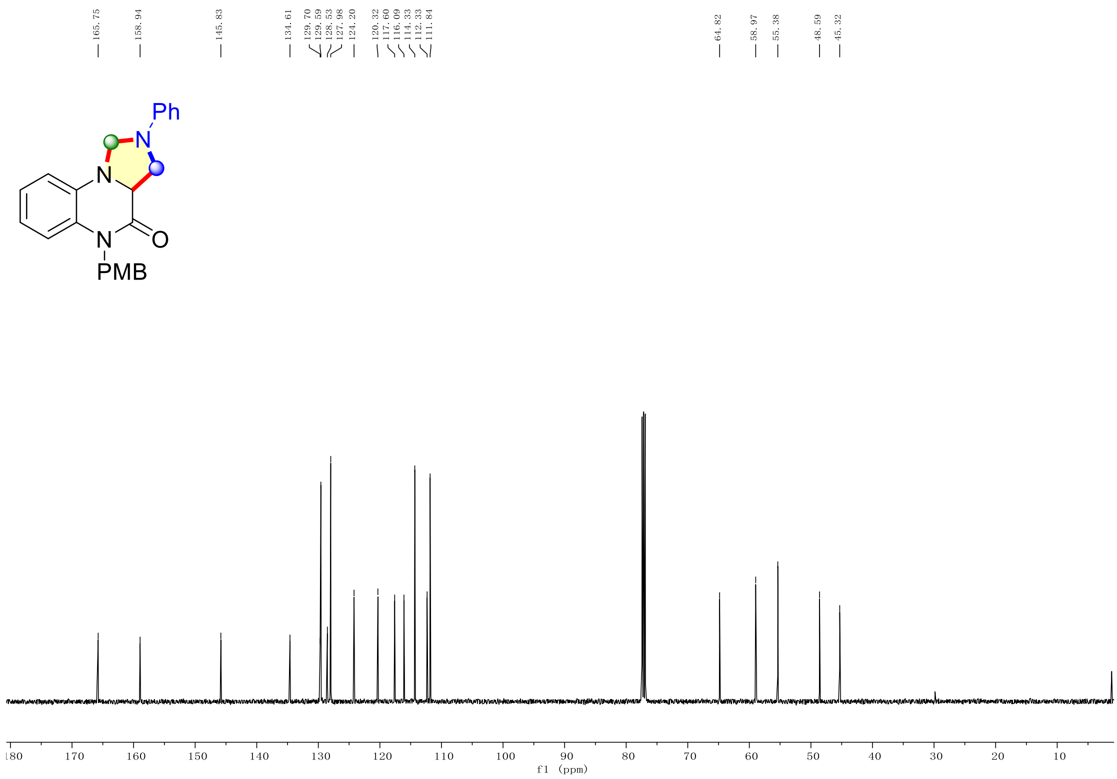




5-(4-methoxybenzyl)-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4fa）

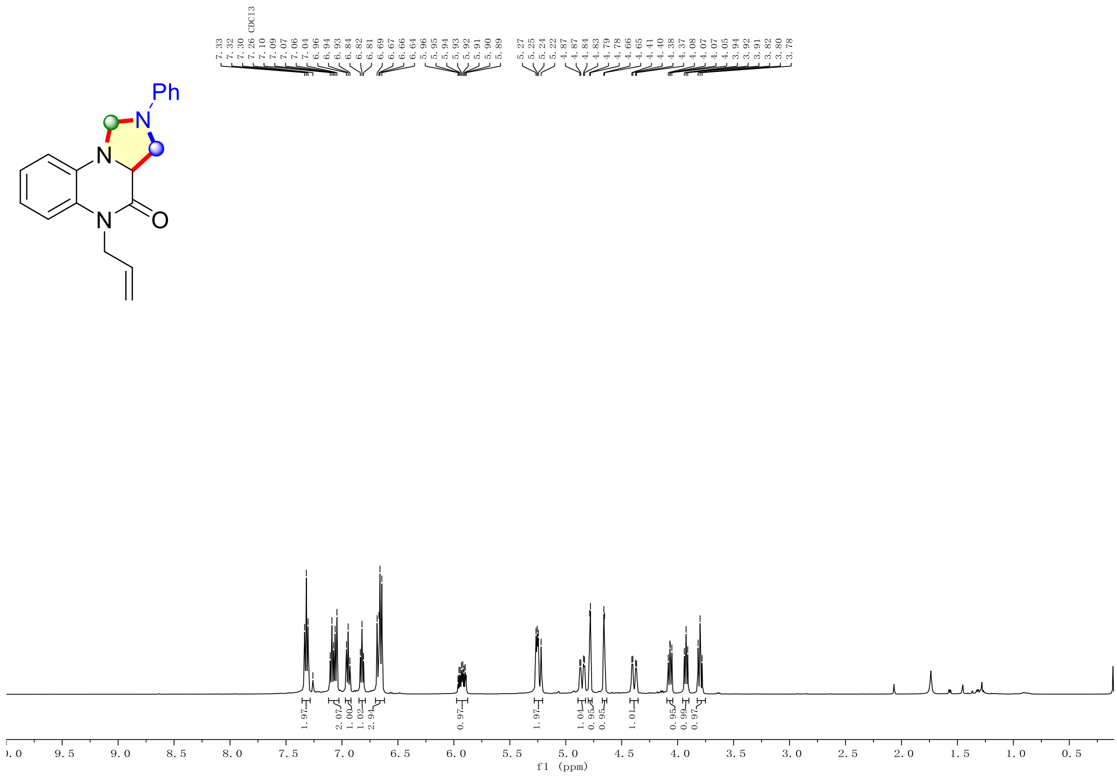
4fa ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

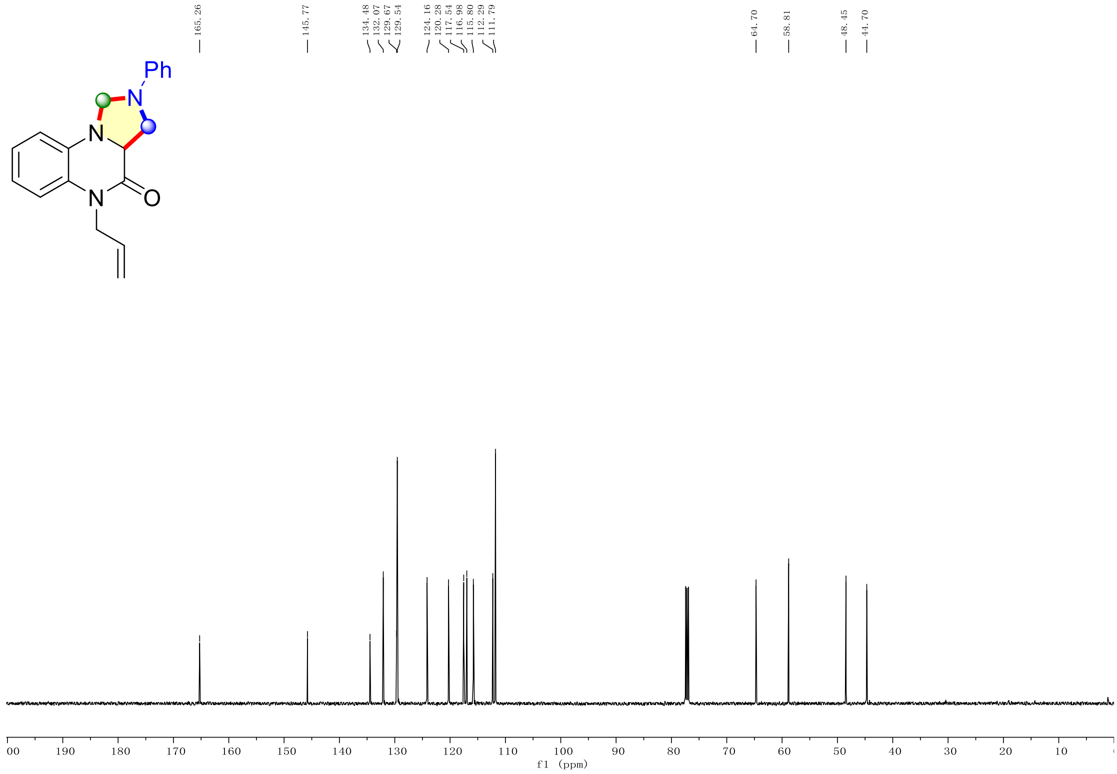




5-allyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4ga）

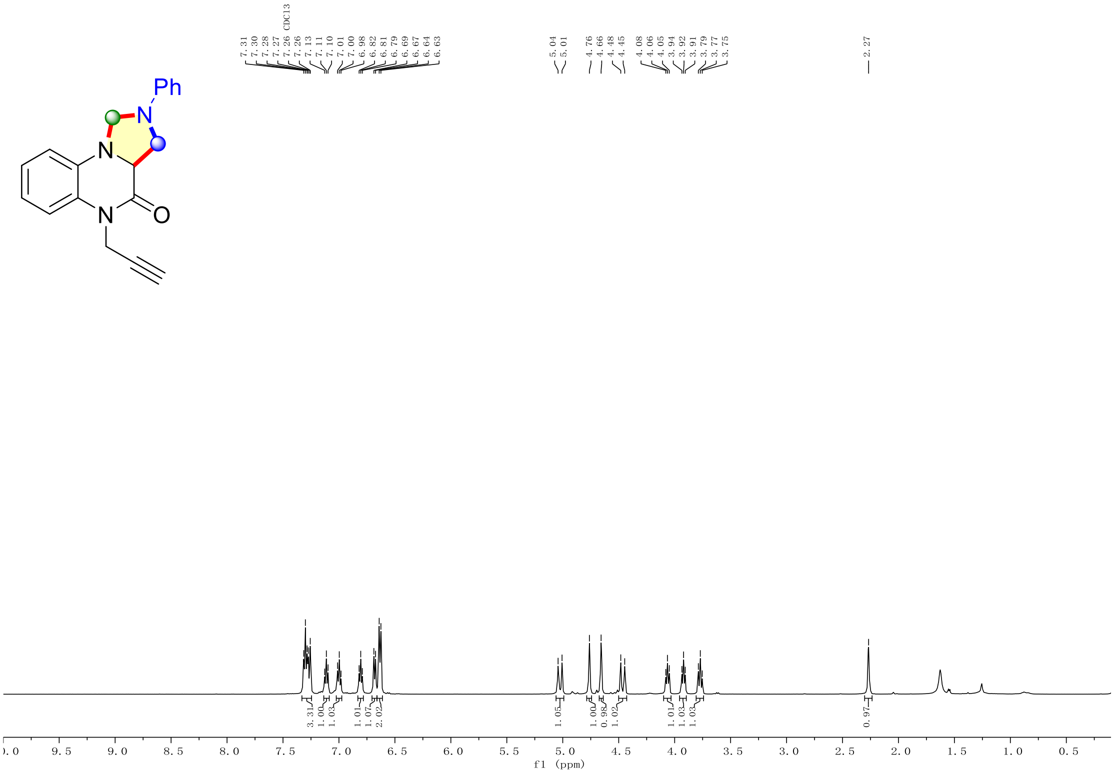
4ga ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

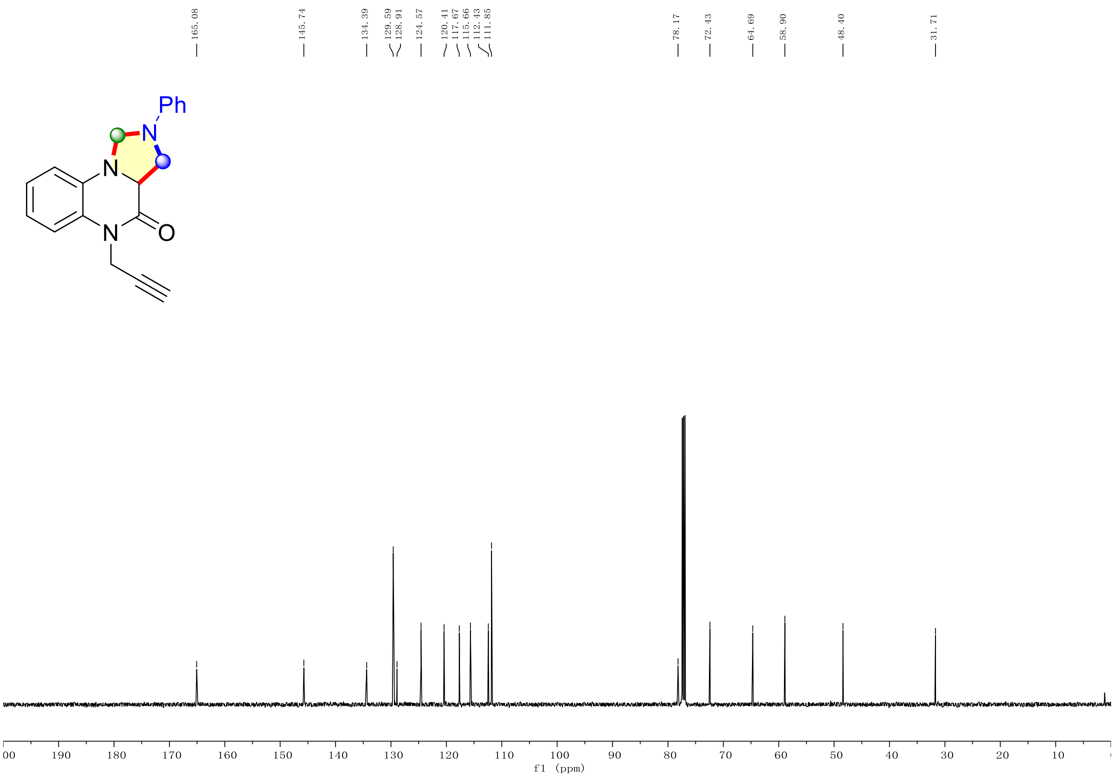




2-phenyl-5-(prop-2-yn-1-yl)-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4ha）

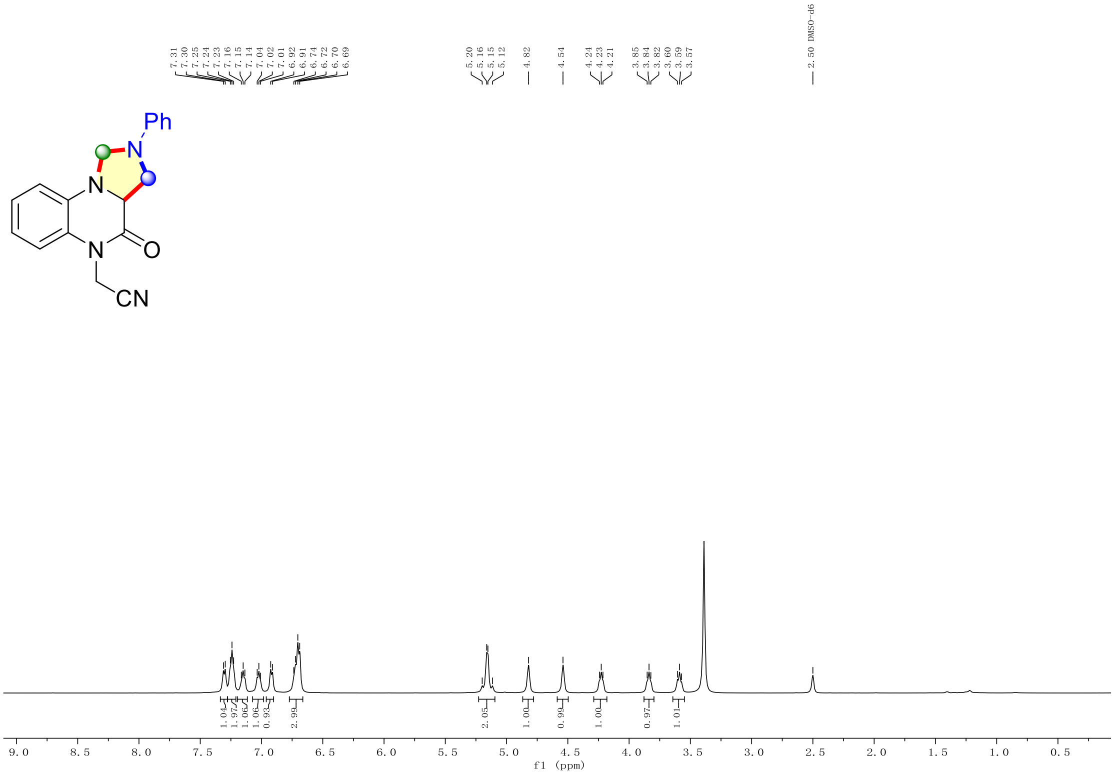
4ha ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

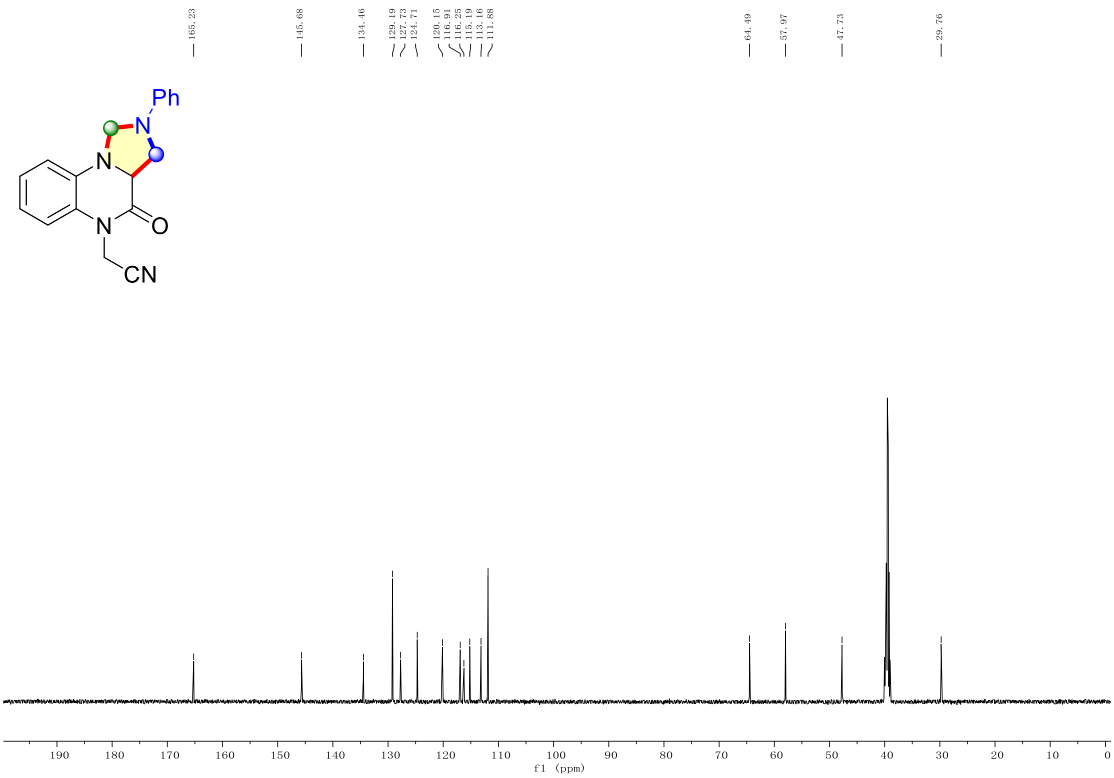




2-(4-oxo-2-phenyl-2,3,3a,4-tetrahydroimidazo[1,5-a]quinoxalin-5(1*H*)-yl)acetonitrile（4ia）

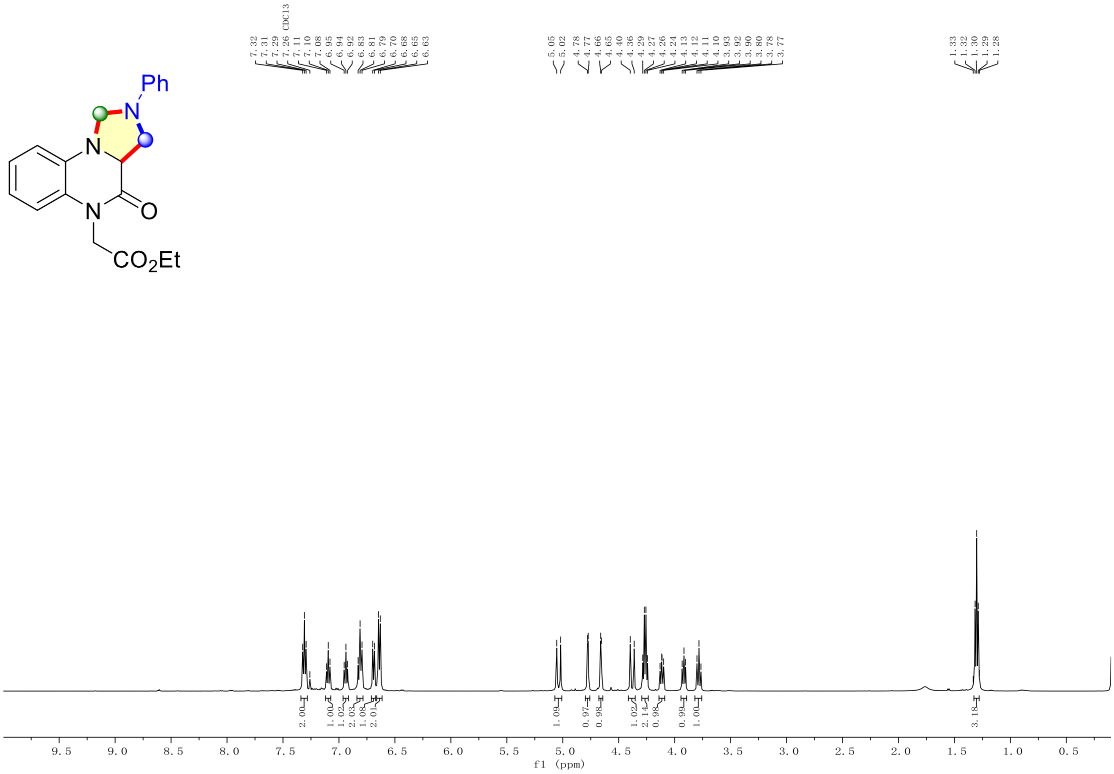
4ia ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

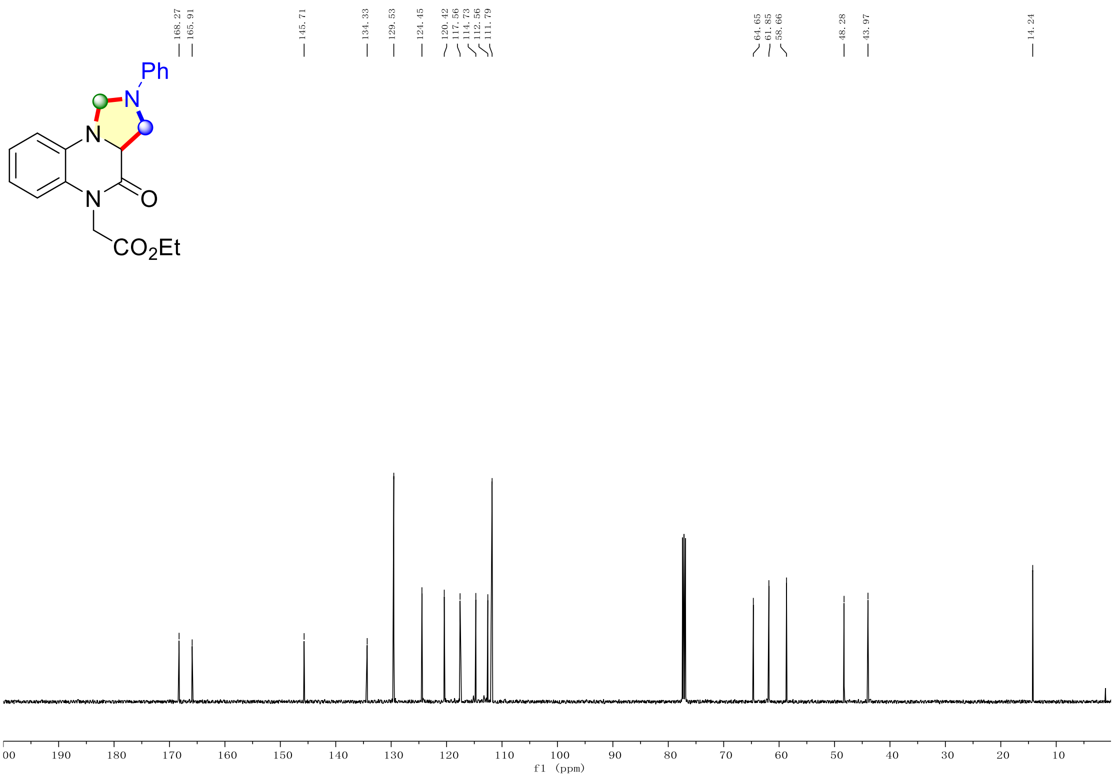




Ethyl-2-(4-oxo-2-phenyl-2,3,3a,4-tetrahydroimidazo[1,5-a]quinoxalin-5(1*H*)-yl)acetate （4ja）

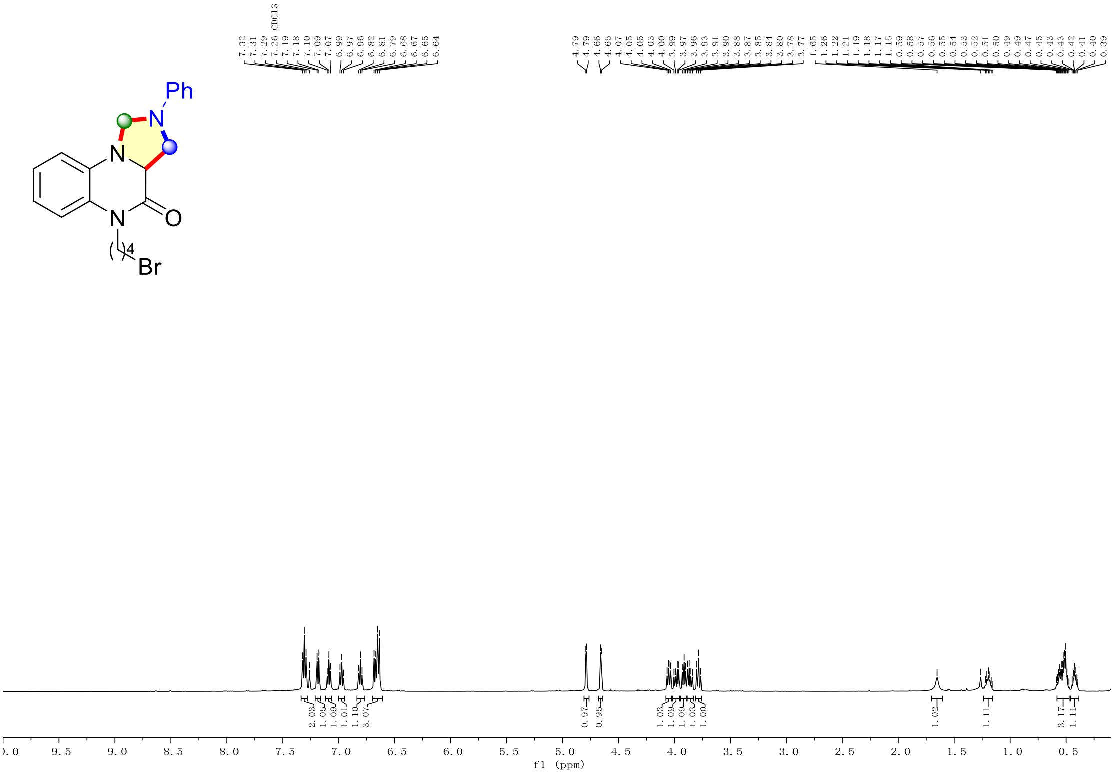
4ja ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

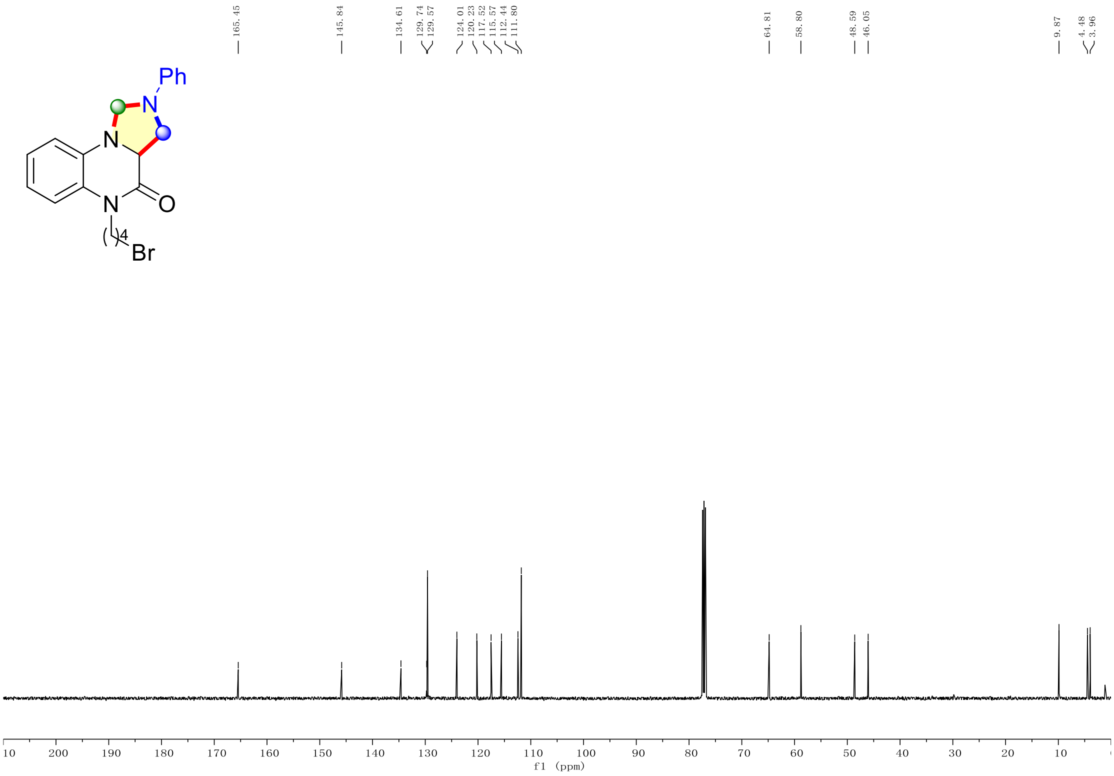




5-(4-bromobutyl)-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4ka）

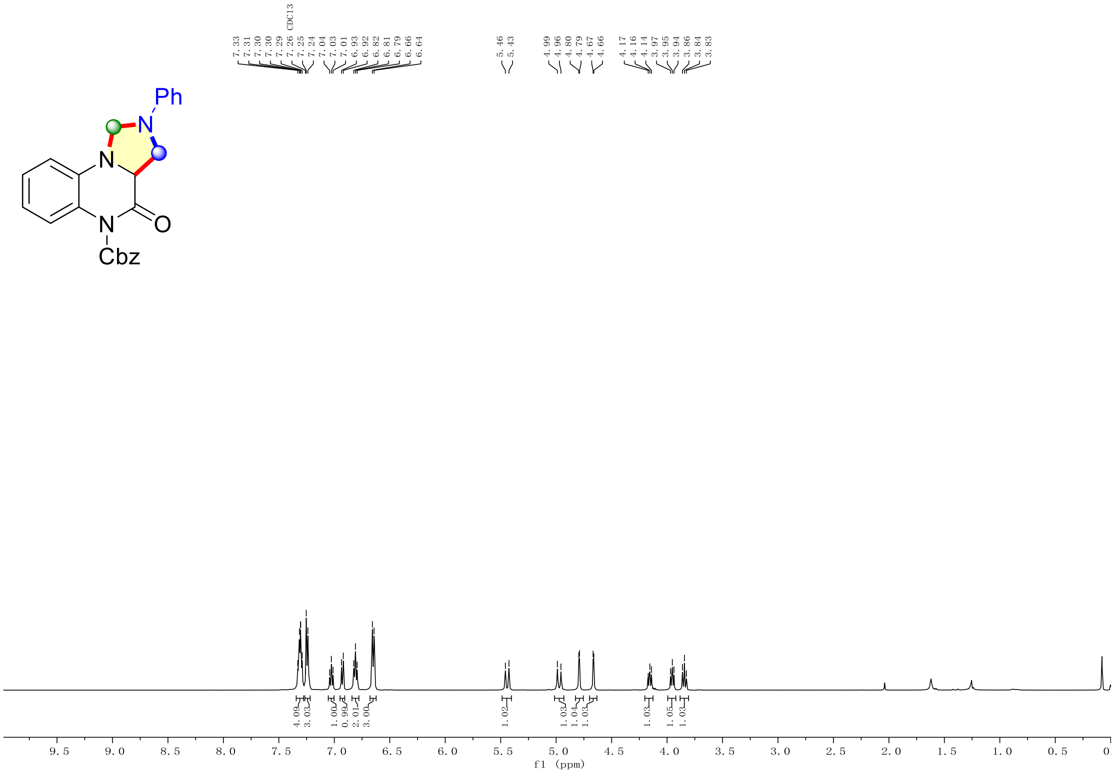
4ka ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

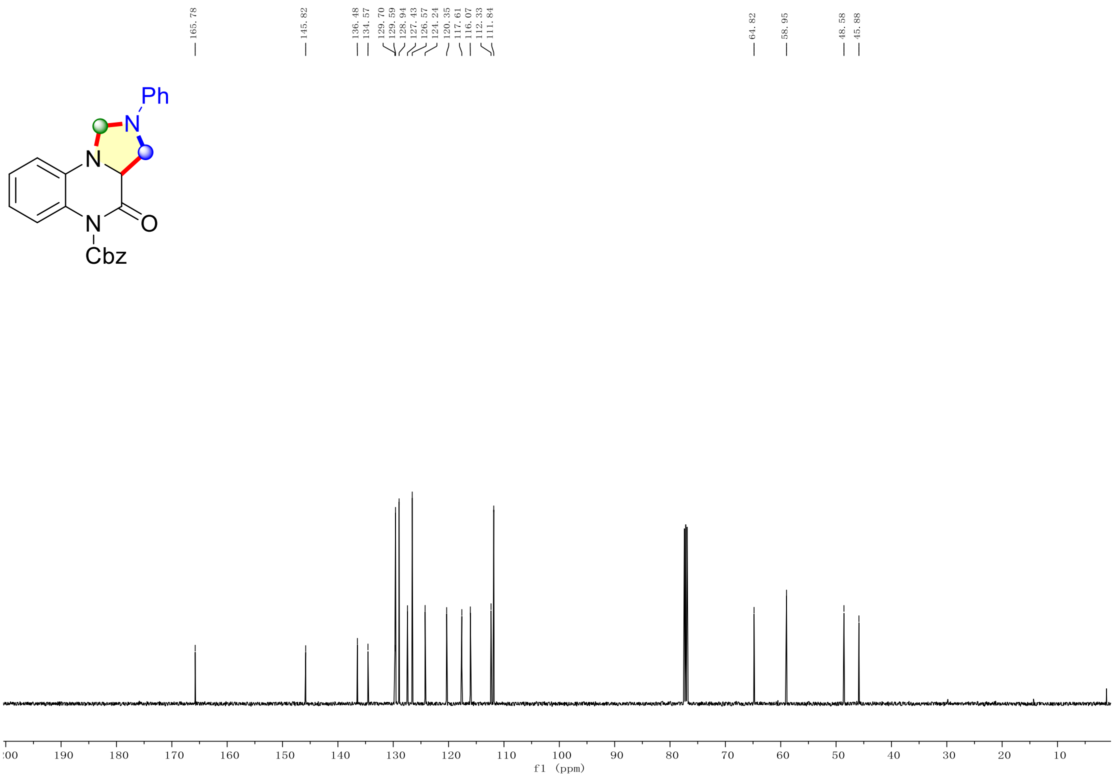




Benzyl(S)-4-oxo-2-phenyl-2,3,3a,4-tetrahydroimidazo[1,5-a]quinoxaline-5(1*H*)-carboxylate（4la）

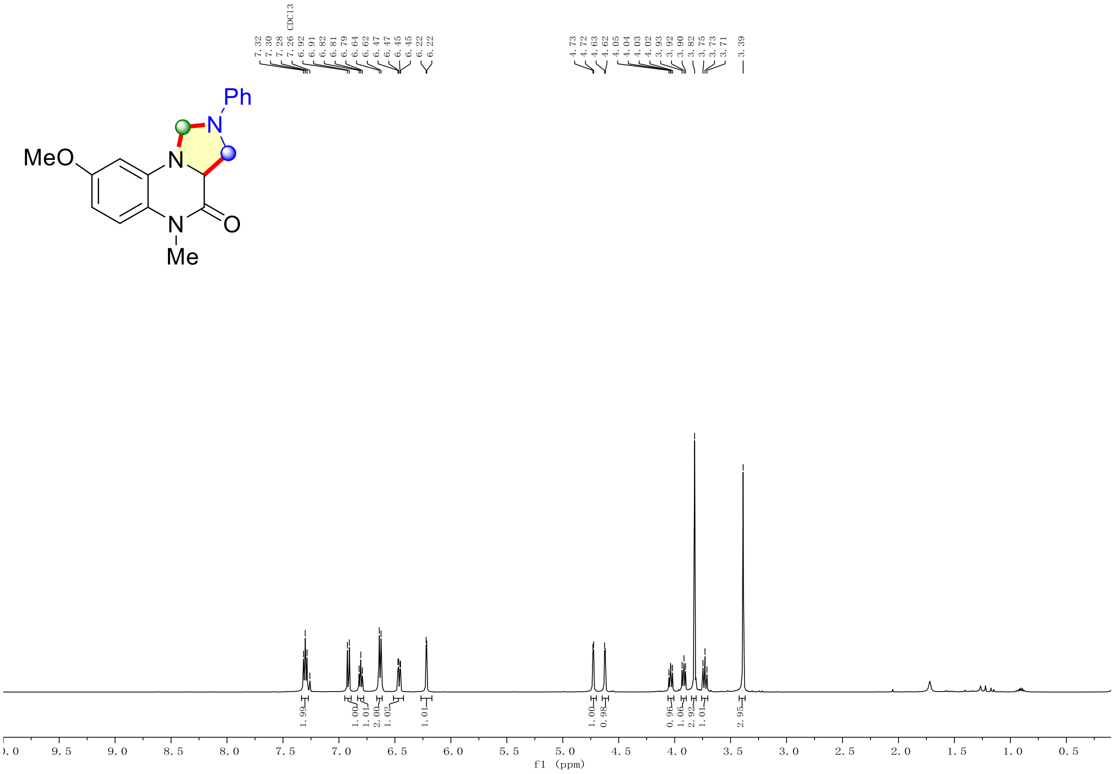
4la ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

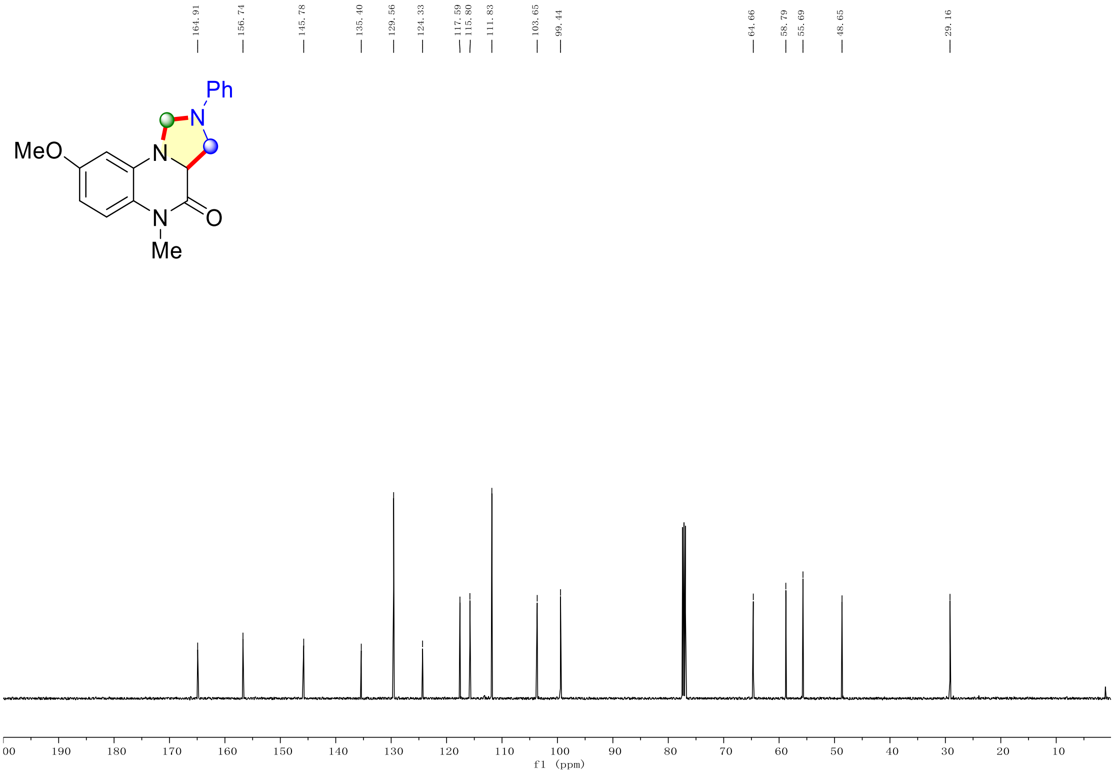




8-methoxy-5-methyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4ma）

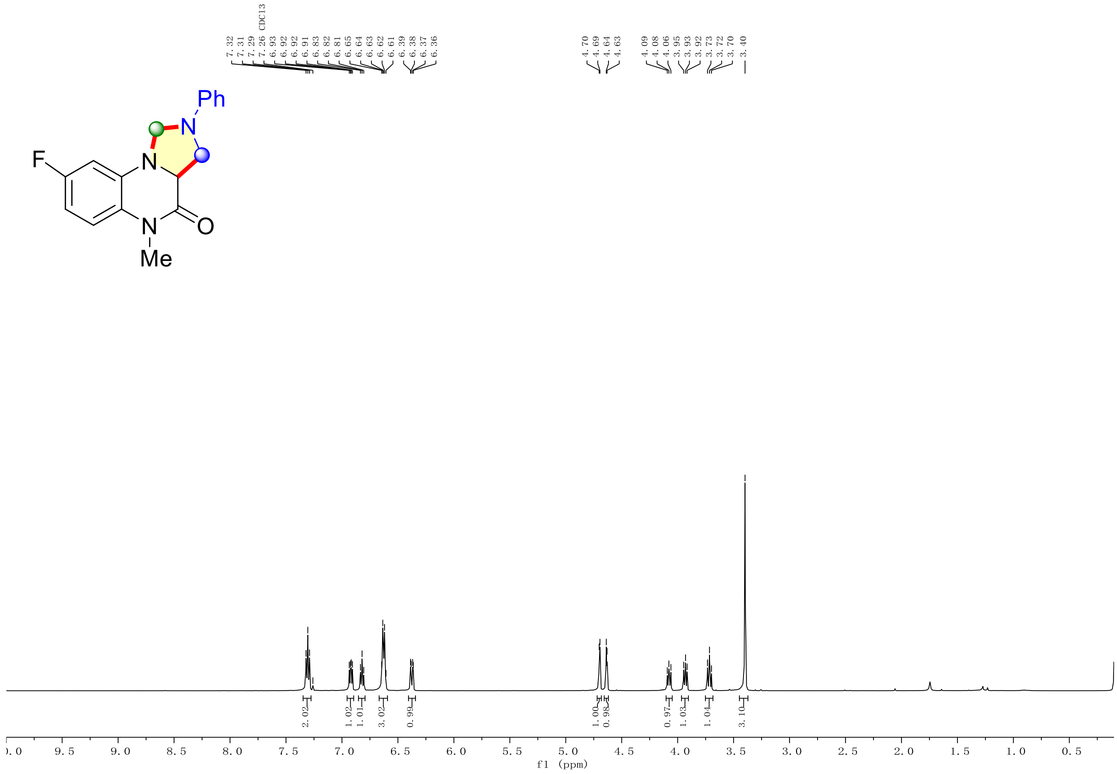
4ma ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

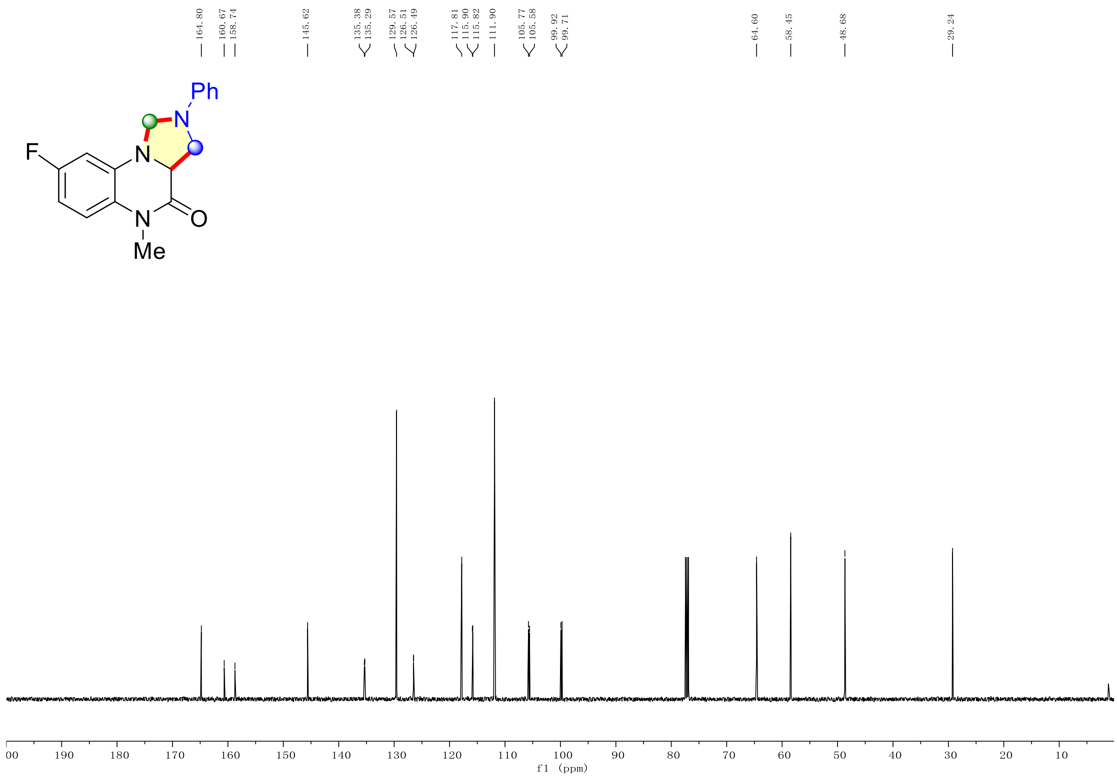




8-fluoro-5-methyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4na）

4na ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz) and ^{19}F NMR (471 MHz)


F
N
Ph
N
N
O
Me
7.32
7.31
7.29
7.26 CDCl3
6.93
6.92
6.92
6.91
6.83
6.82
6.81
6.65
6.64
6.63
6.62
6.61
6.39
6.38
6.37
6.36
4.70
4.69
4.64
4.63
4.09
4.08
4.06
3.95
3.93
3.92
3.73
3.72
3.70
3.40
2.02
1.02
1.01
3.02
0.99
1.00
0.98
0.97
1.03
1.04
3.10
f1 (ppm)


164.80
160.67
158.74
145.62
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135.29
129.57
126.51
126.49
117.81
115.90
115.82
111.90
105.77
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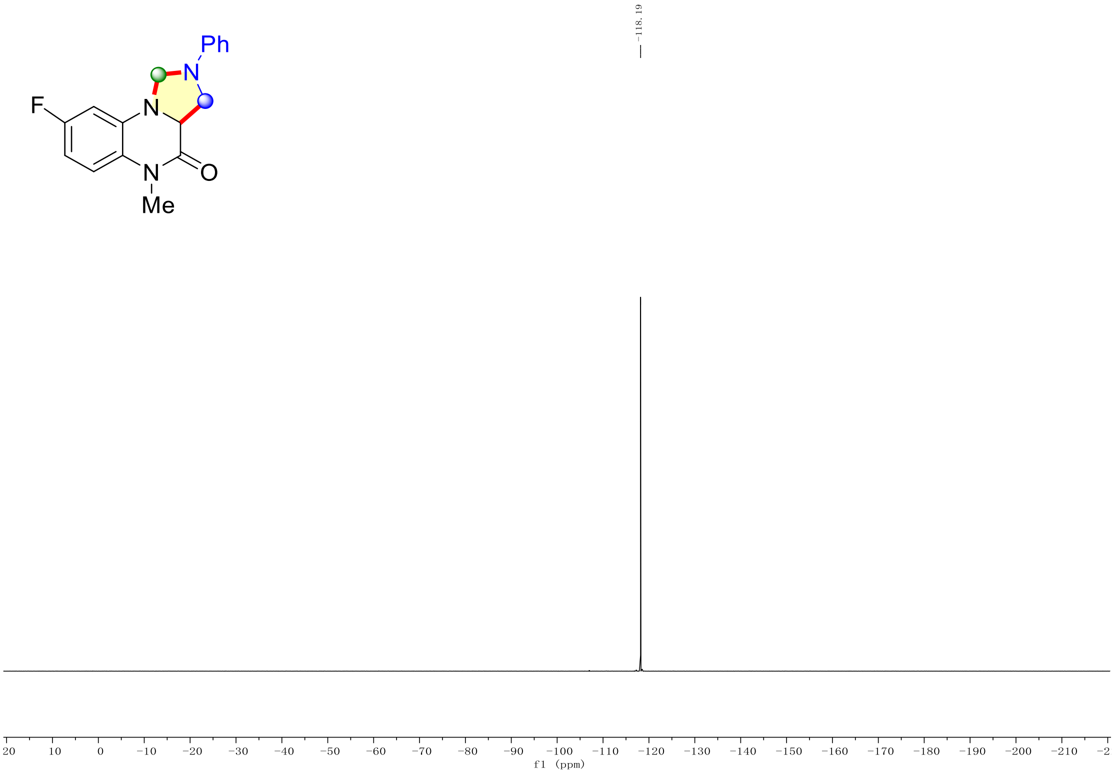
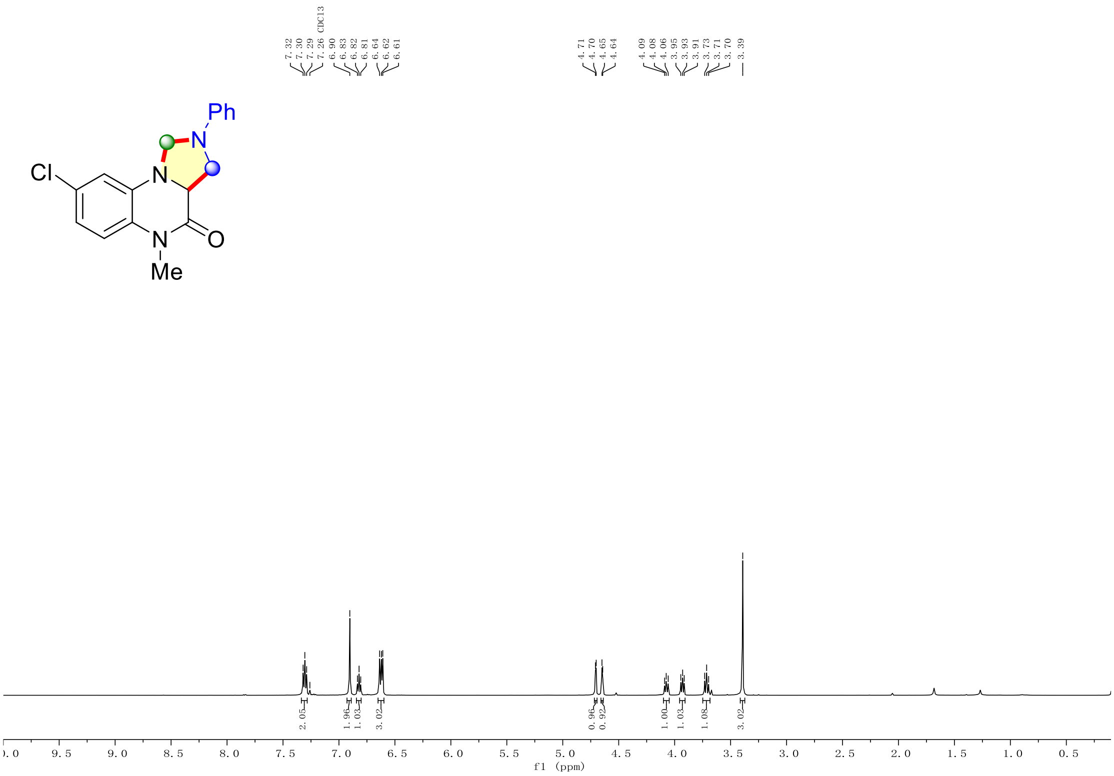
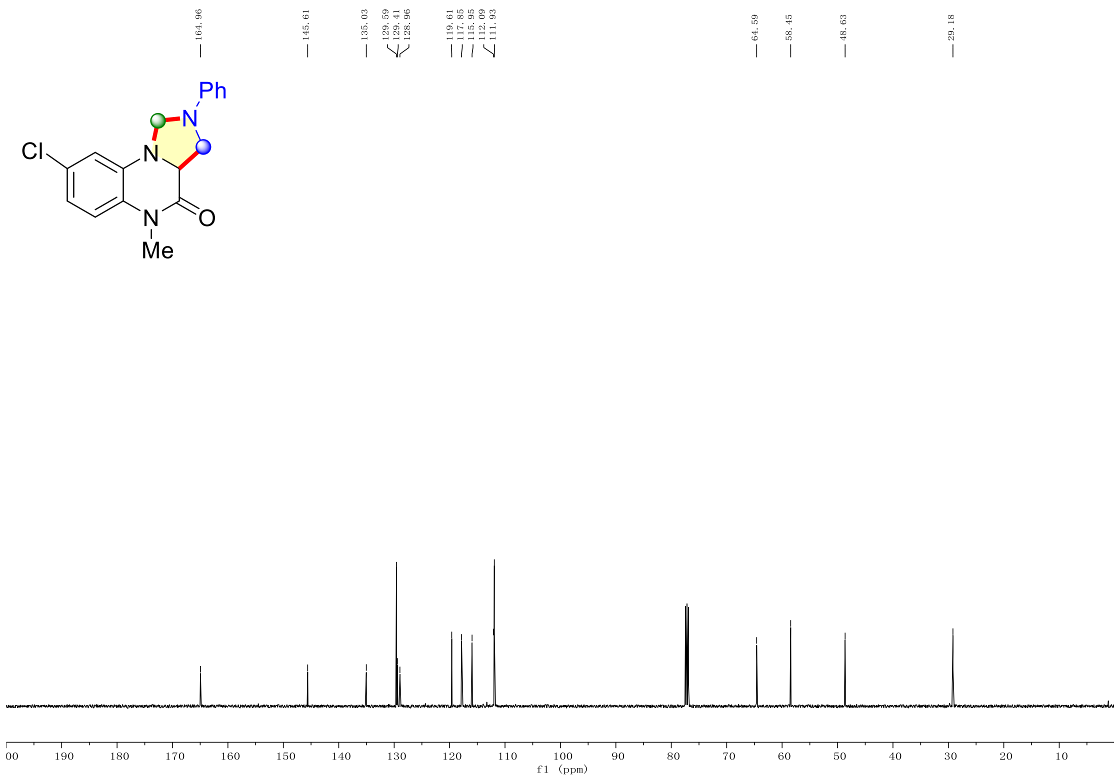
99.92
99.71
64.60
58.45
48.68
29.24
F
N
Ph
N
N
O
Me
f1 (ppm)



8-chloro-5-methyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H)*-one（4oa）

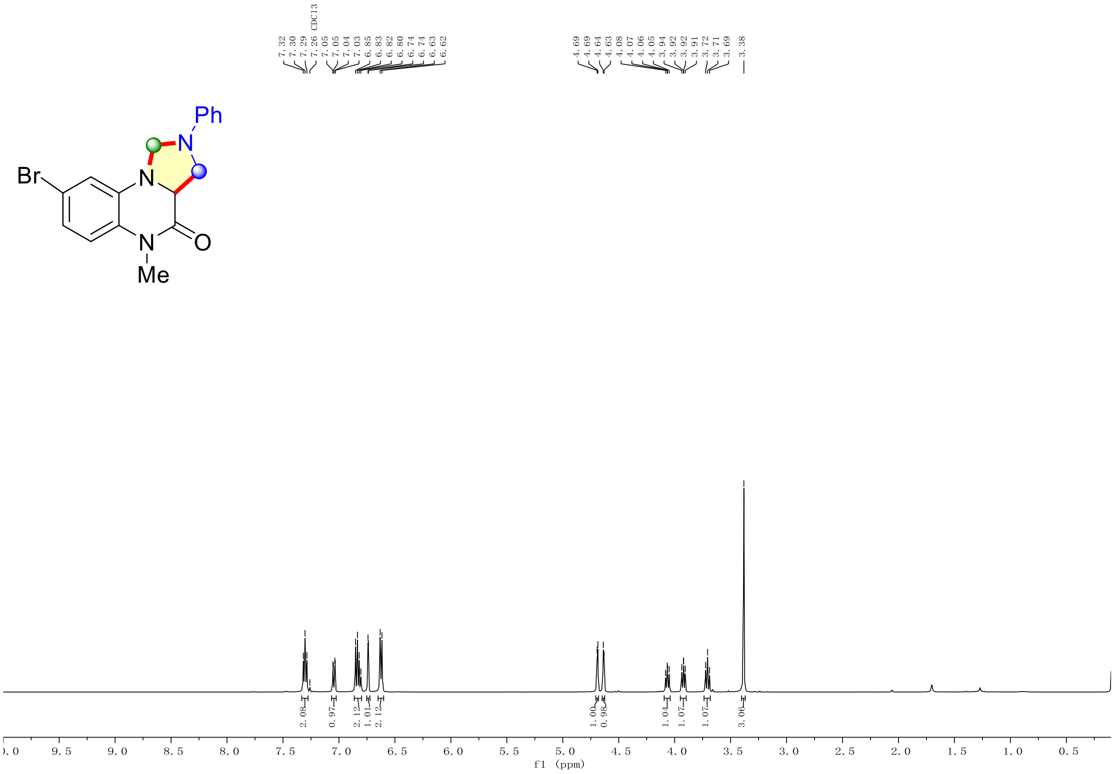
4oa ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

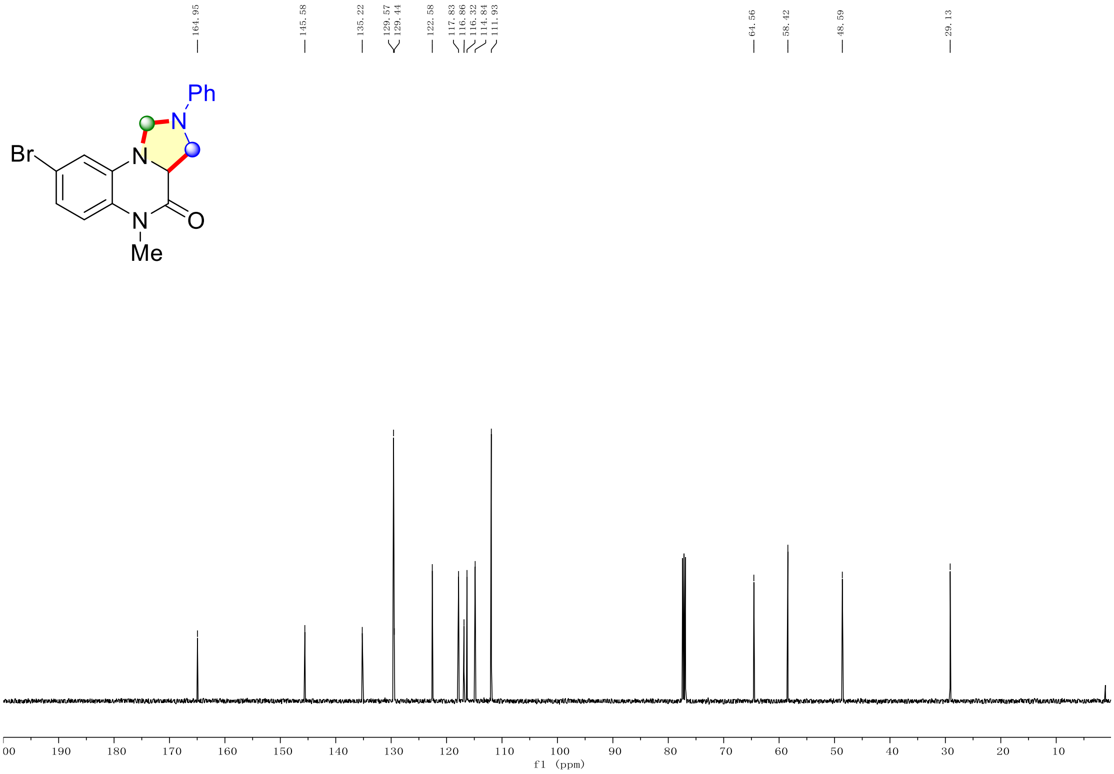




8-bromo-5-methyl-2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4pa）

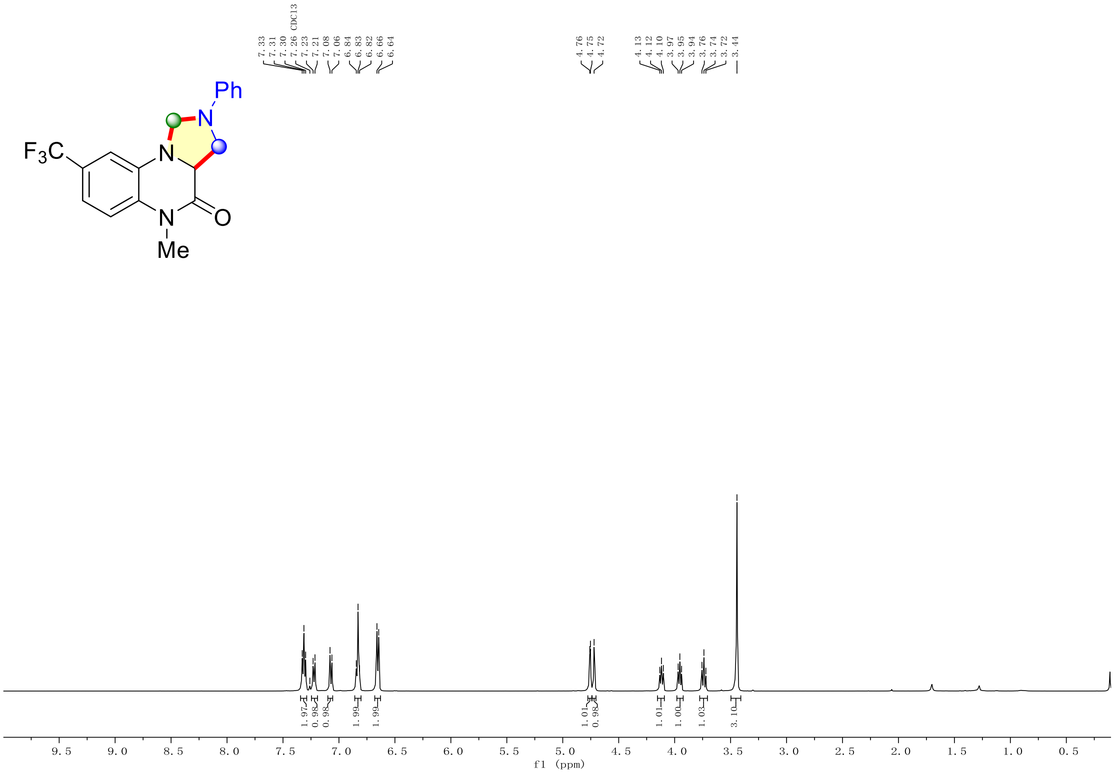
4pa ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

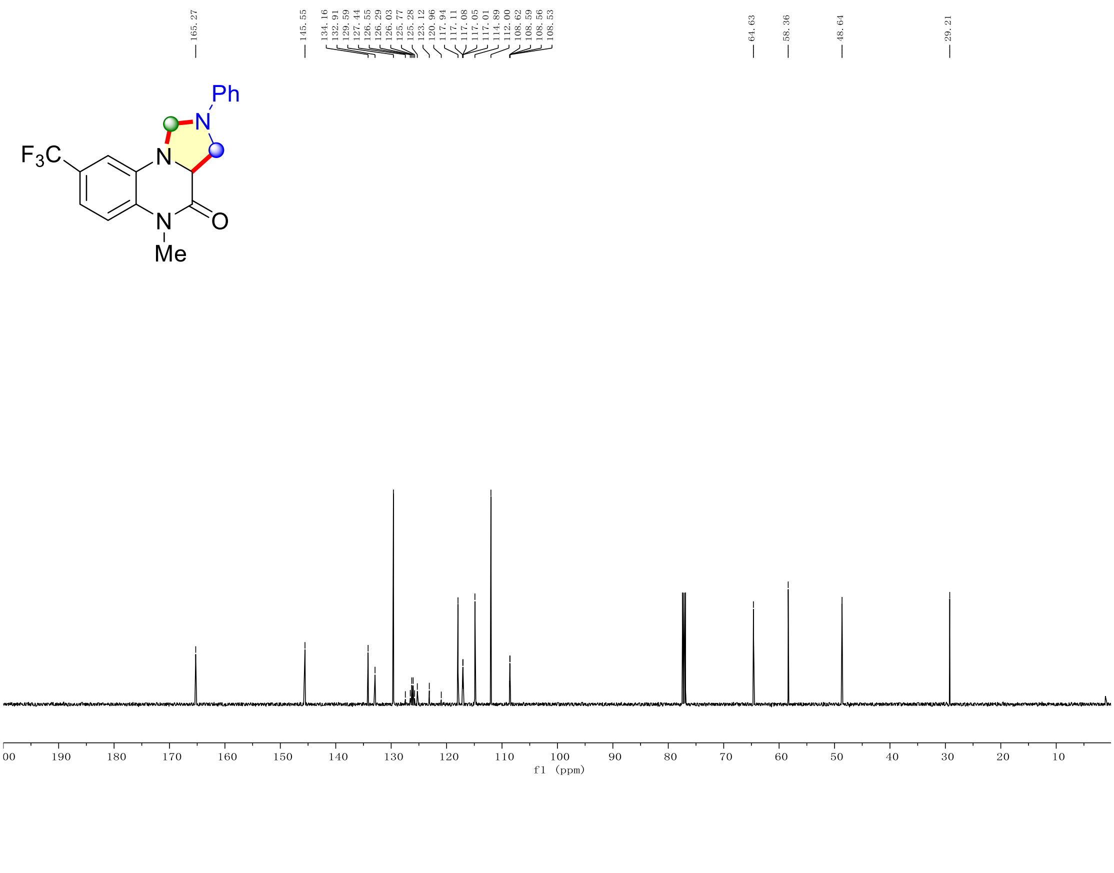


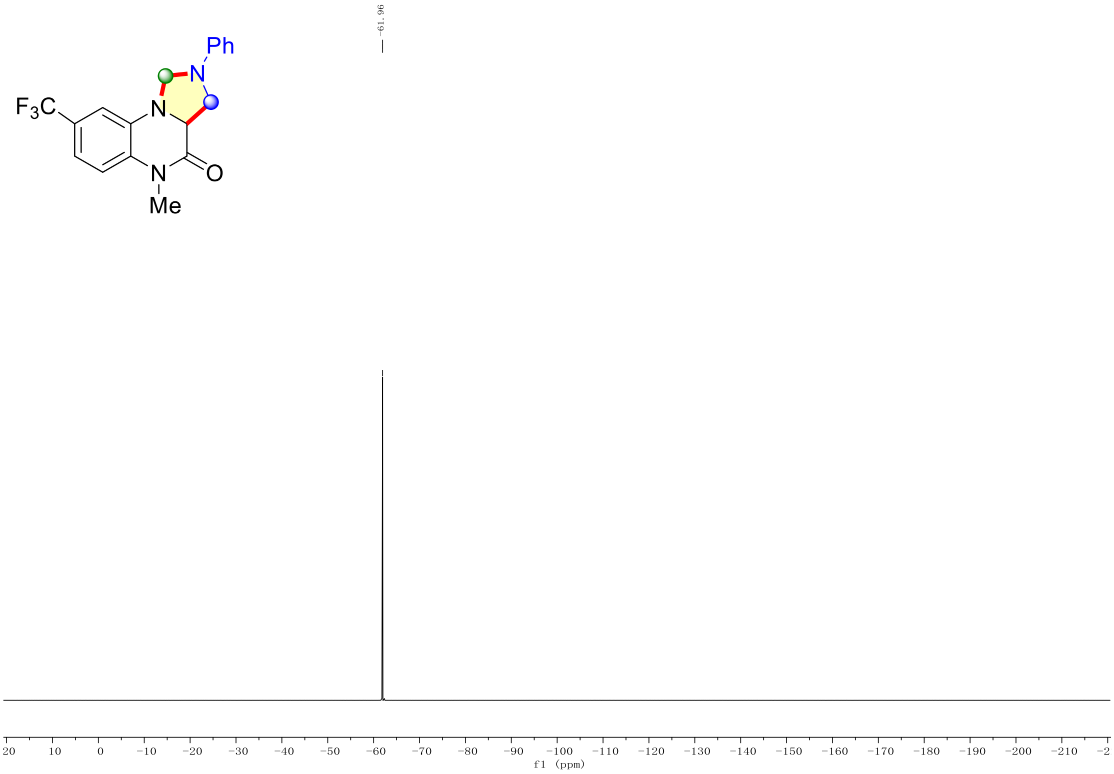


5-methyl-2-phenyl-8-(trifluoromethyl)-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4qa）

4qa ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz) and ^{19}F NMR (471 MHz)

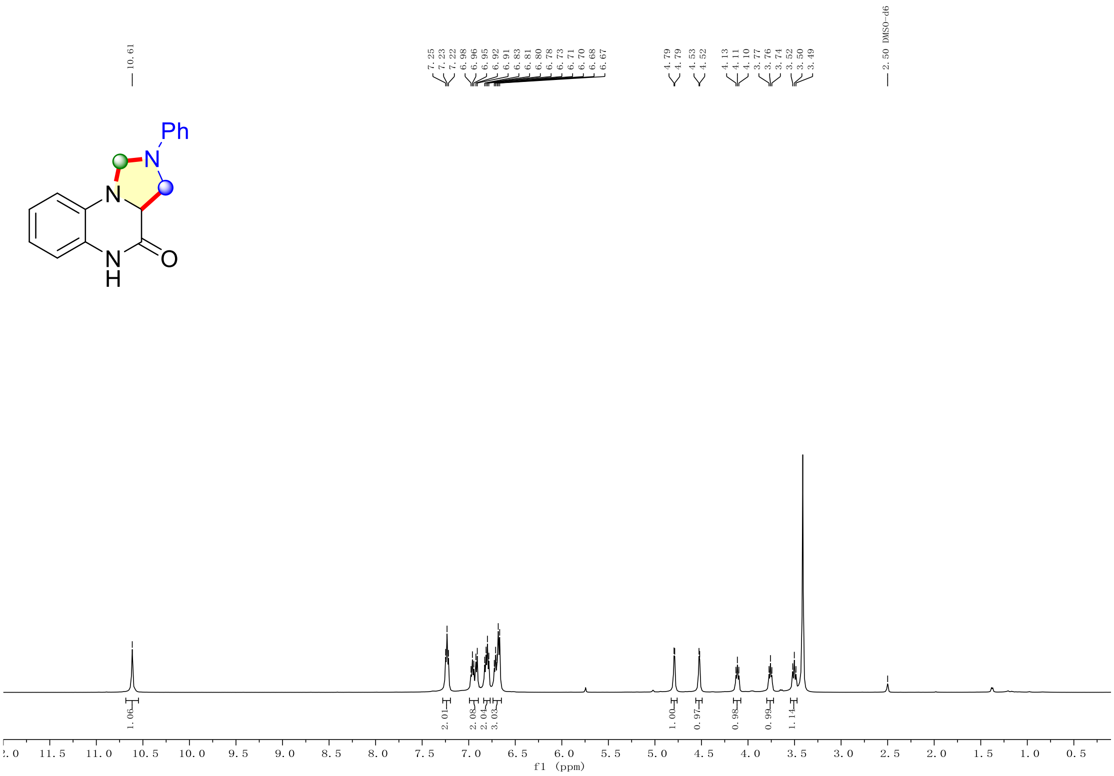


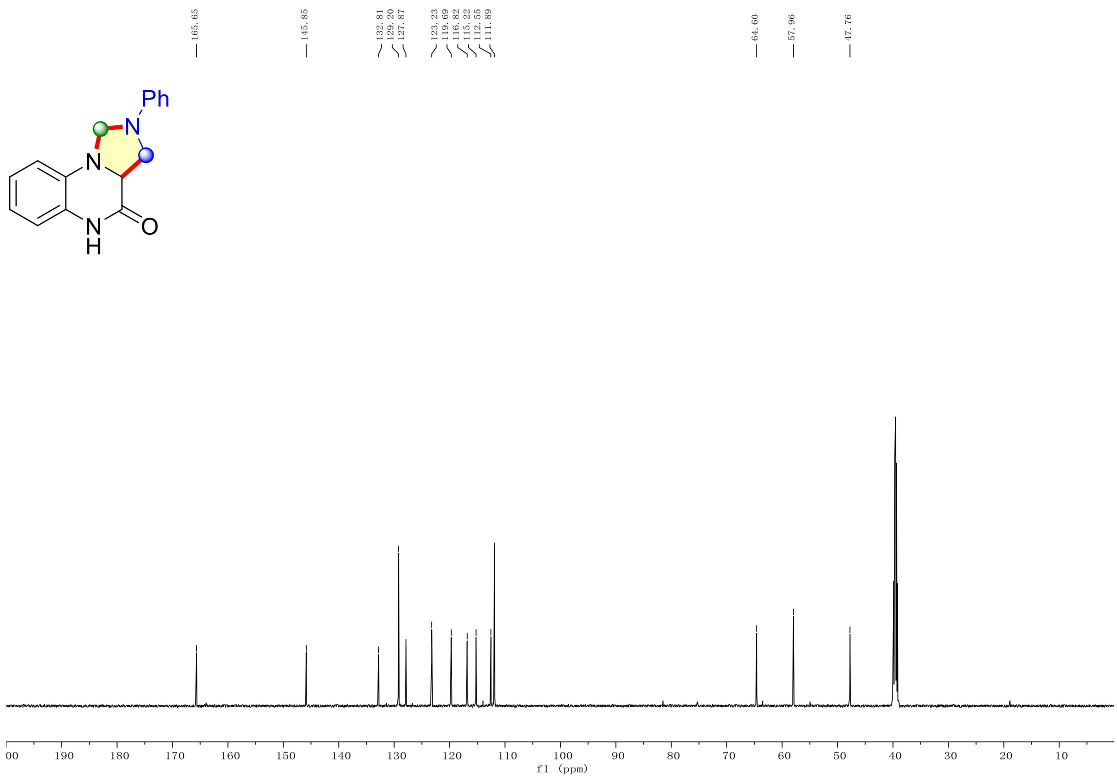




2-phenyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4ra）

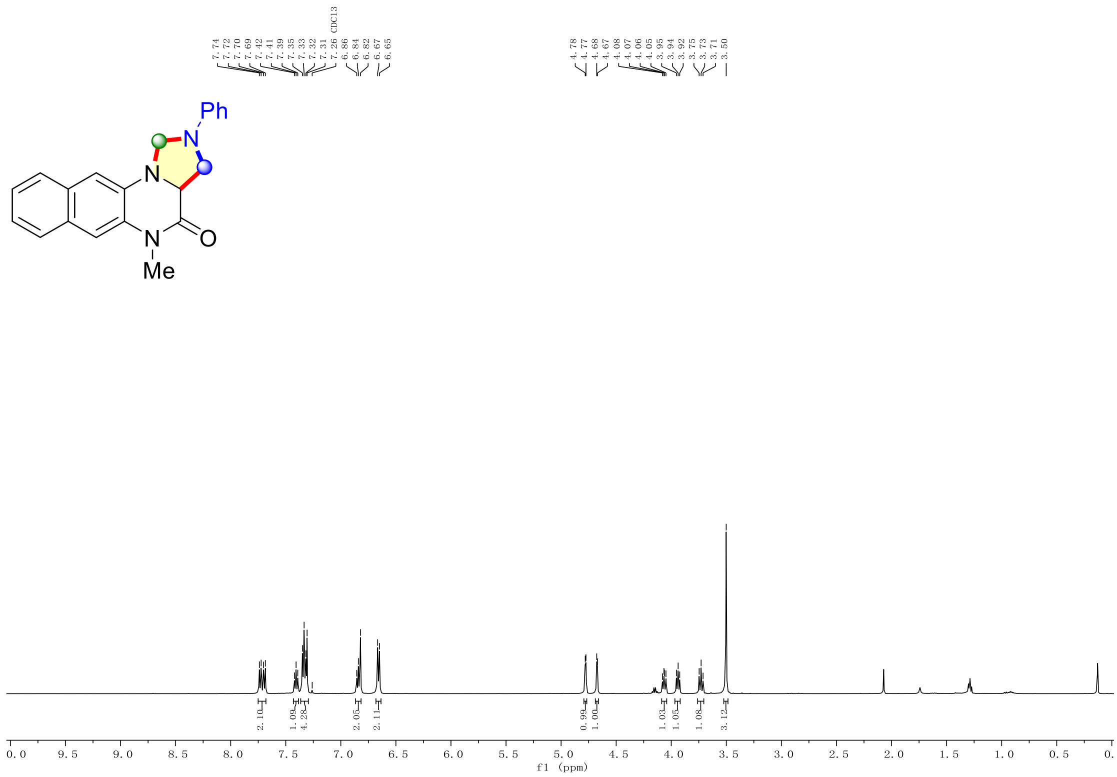
4ra ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

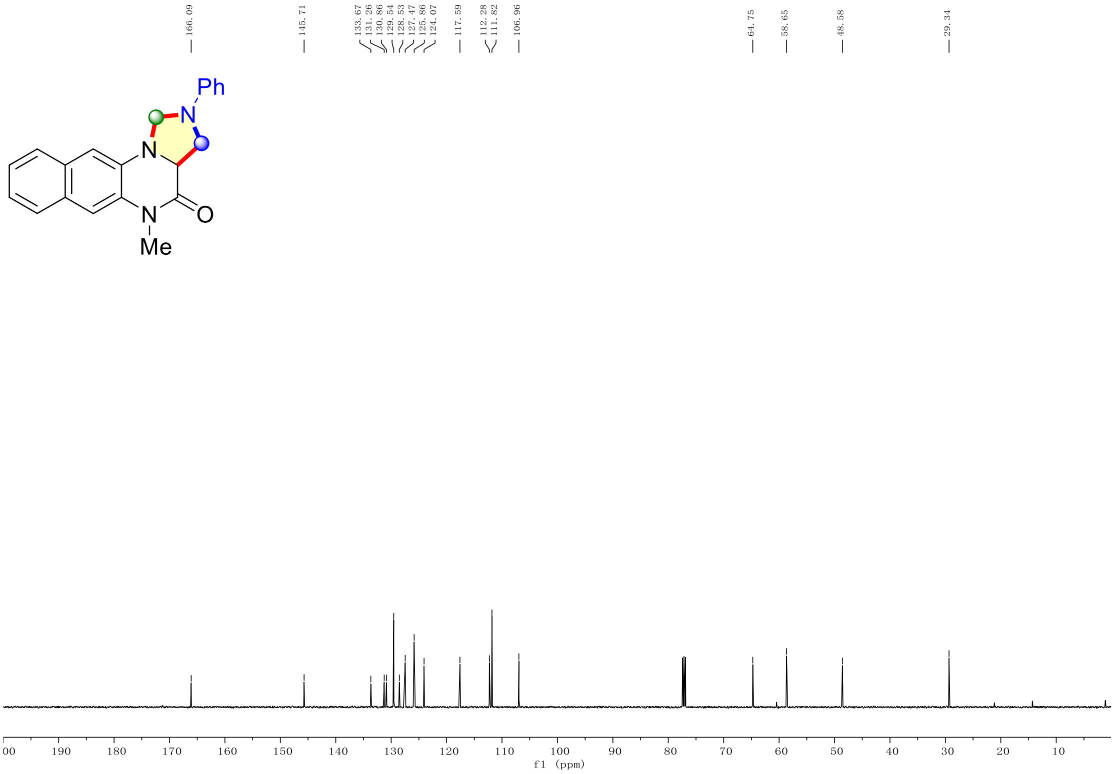




5-methyl-2-phenyl-1,2,3,3a-tetrahydrobenzo[g]imidazo[1,5-a]quinoxalin-4(5*H*)-one（4sa）

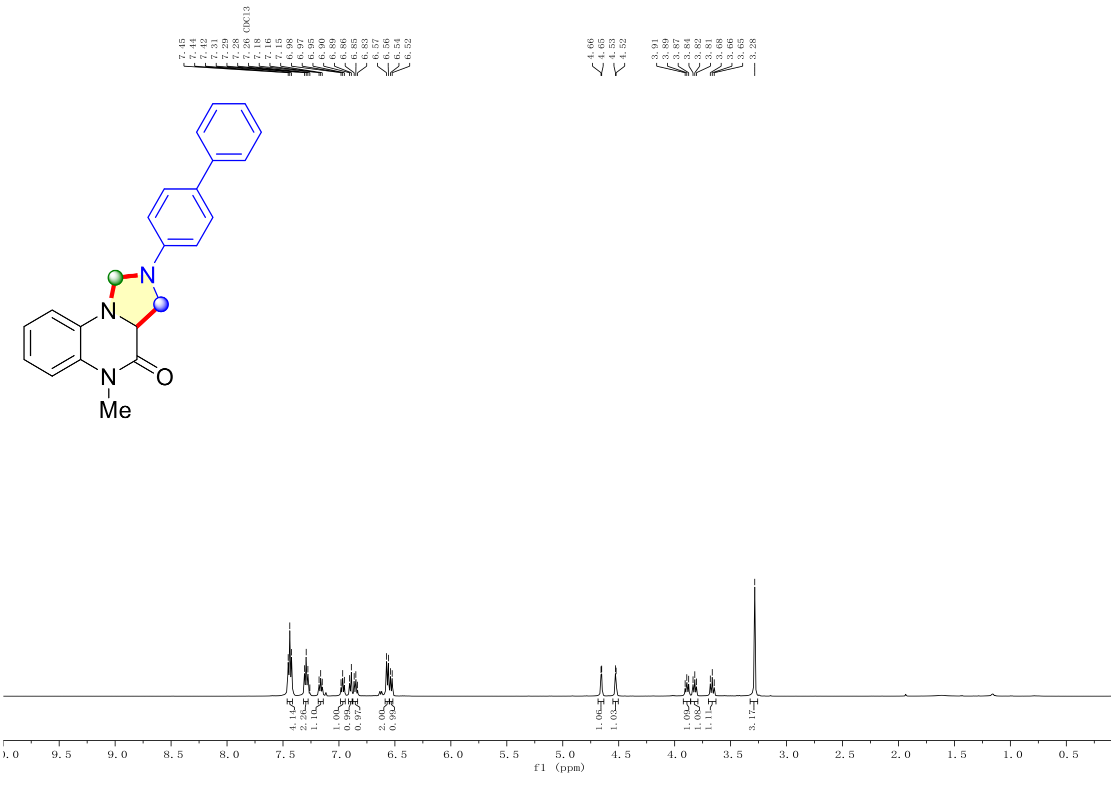
4sa ^{1}HNMR (500 MHz) and ^{13}C NMR (126 MHz)

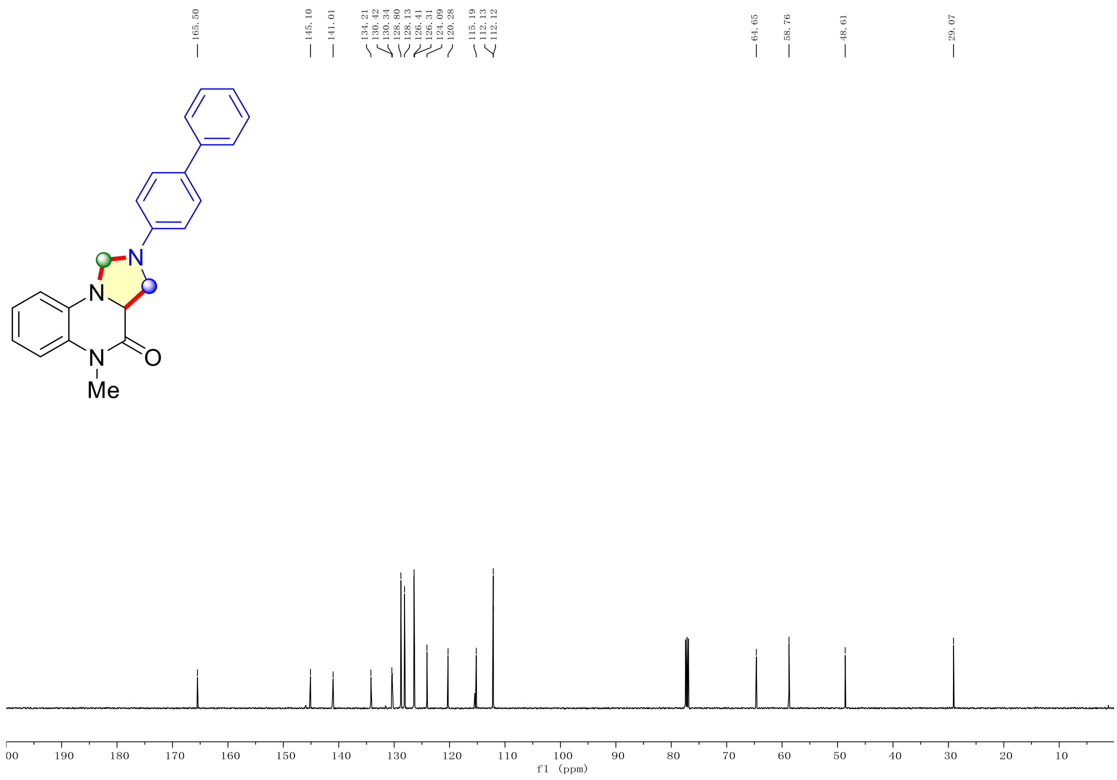




2-([1,1'-biphenyl]-4-yl)-5-methyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4ab）

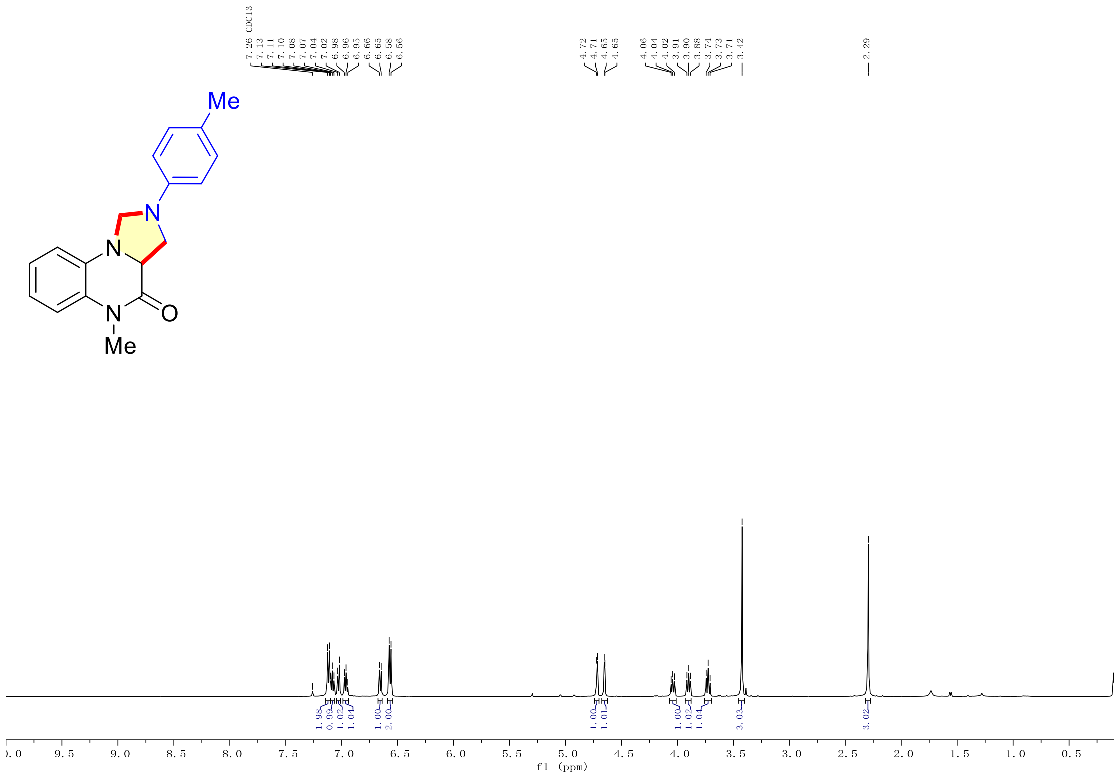
4ab ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

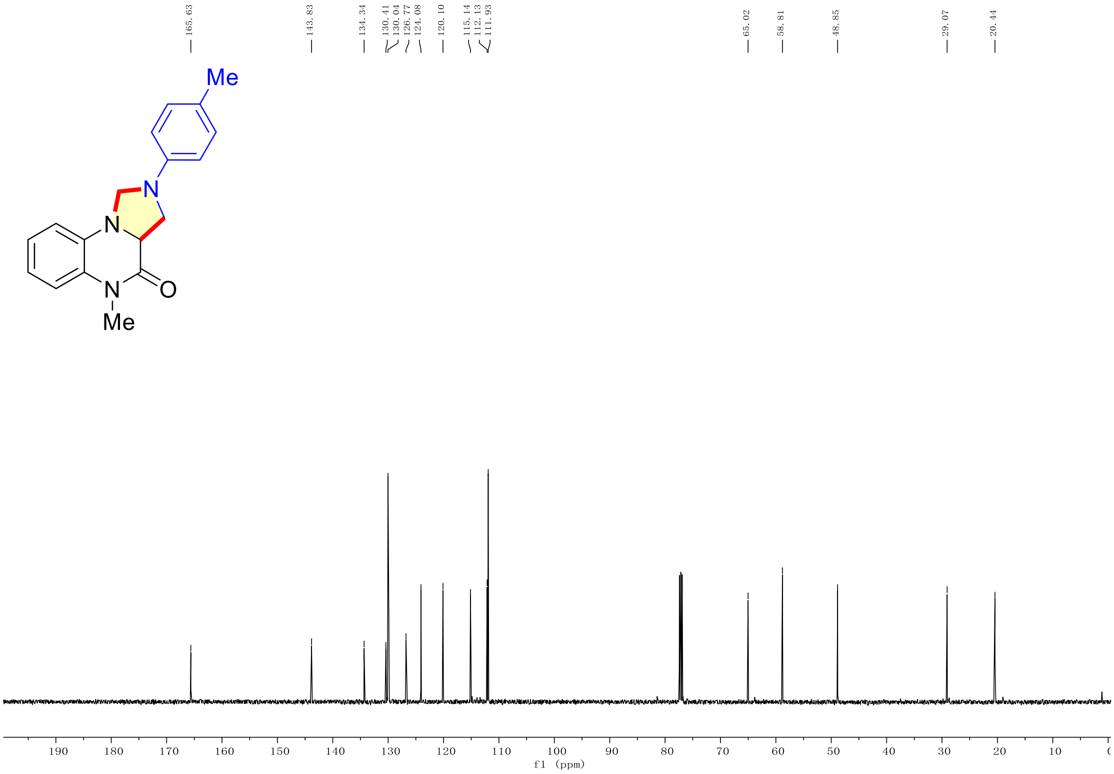




5-methyl-2-(p-tolyl)-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one （4ac）

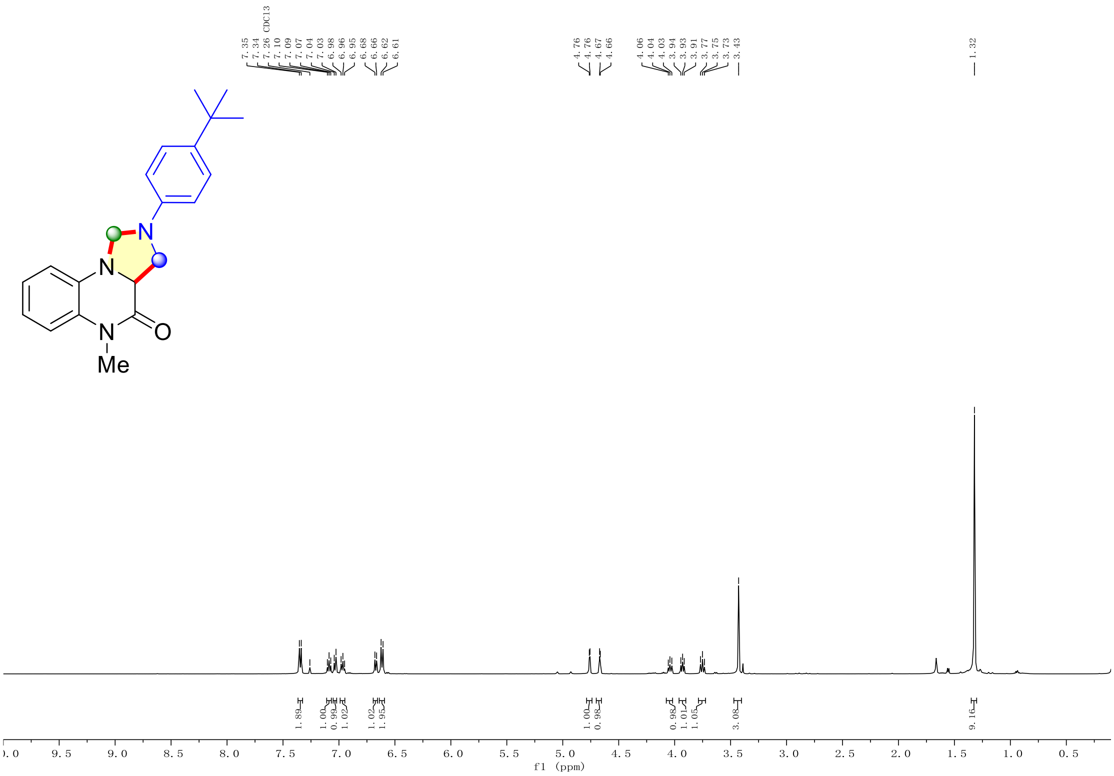
4ac ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

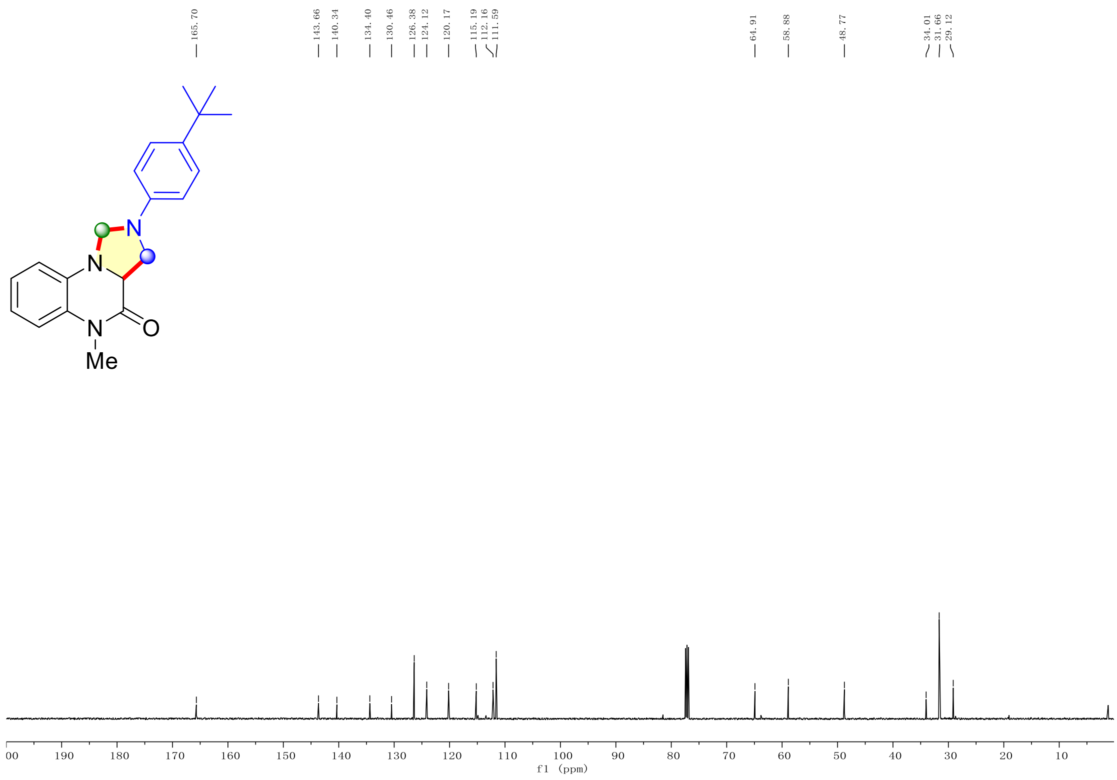




2-(4-(tert-butyl)phenyl)-5-methyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4ad）

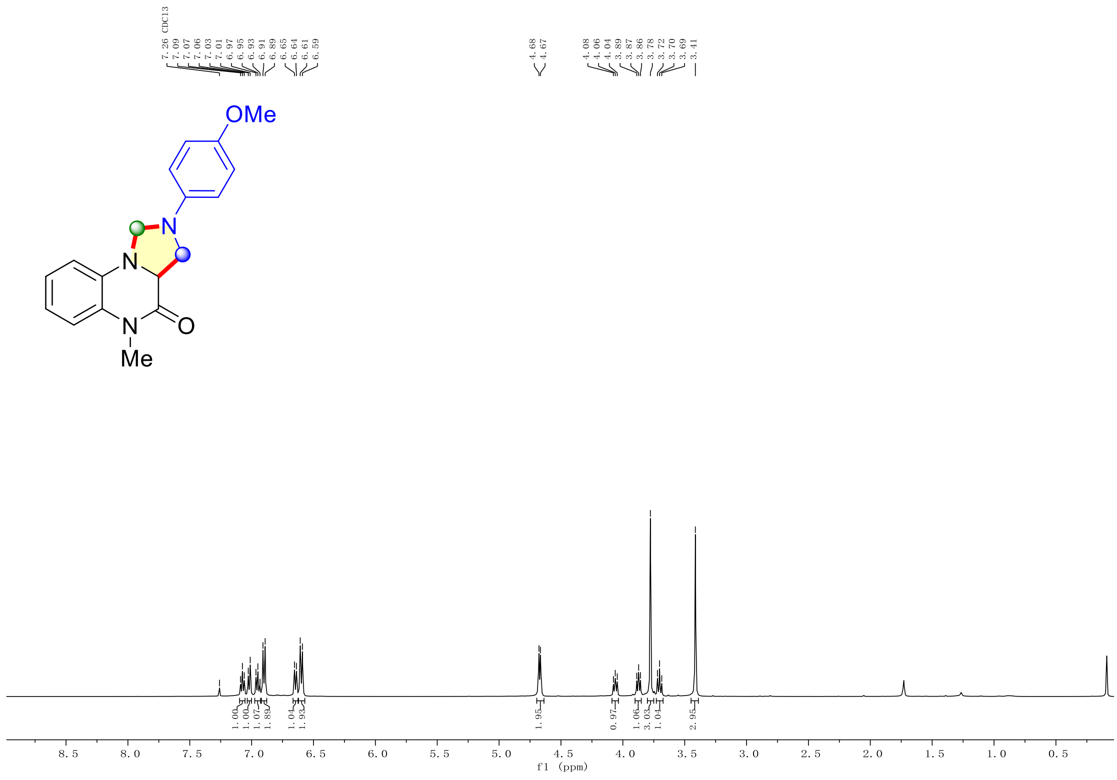
4ad [1]H NMR (500 MHz) and [13]C NMR (126 MHz)

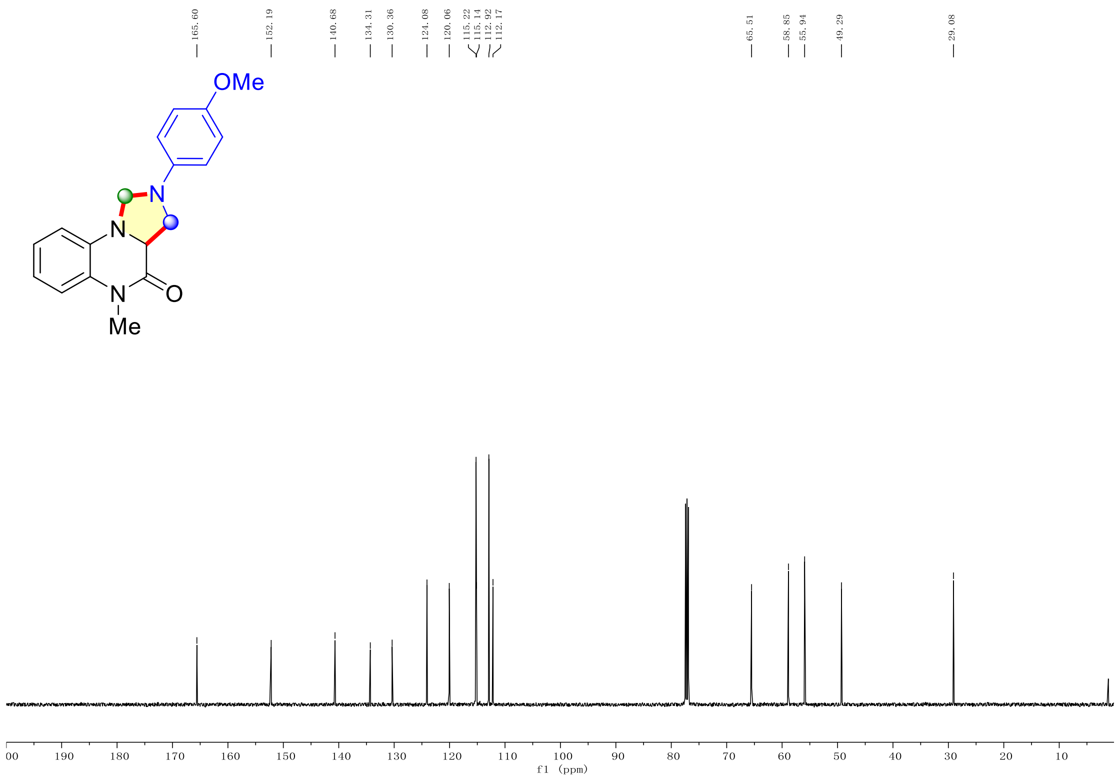




2-(4-methoxyphenyl)-5-methyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4ae）

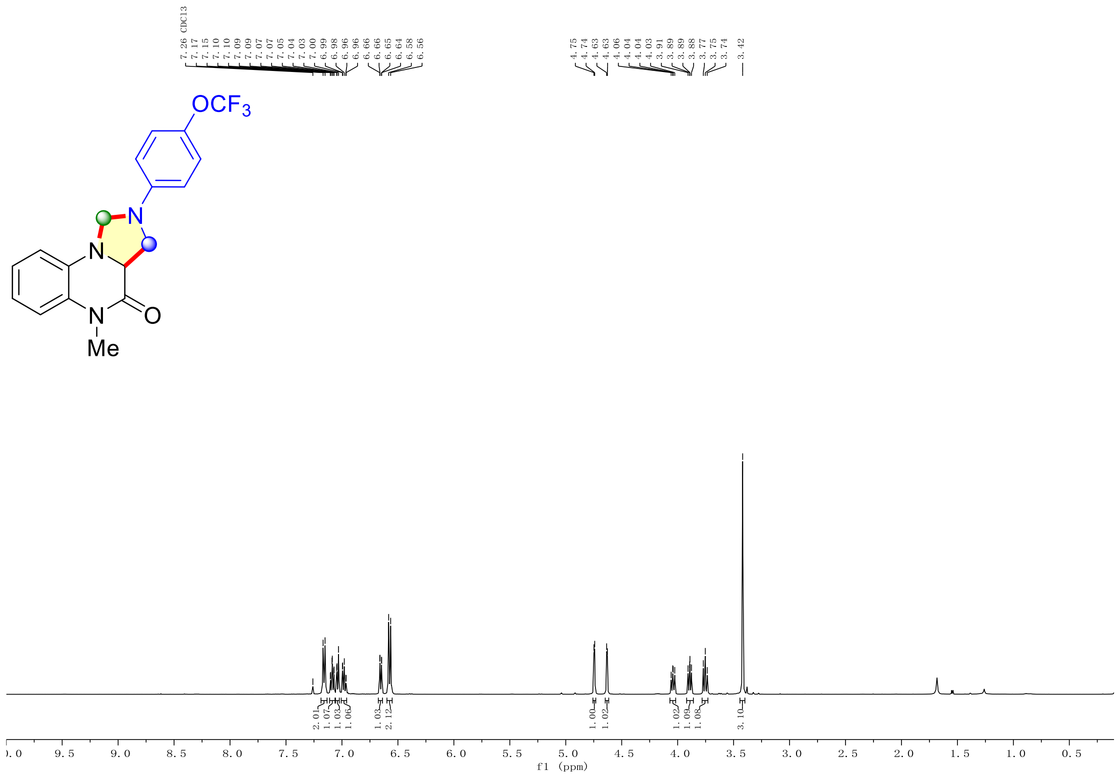
4ae ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

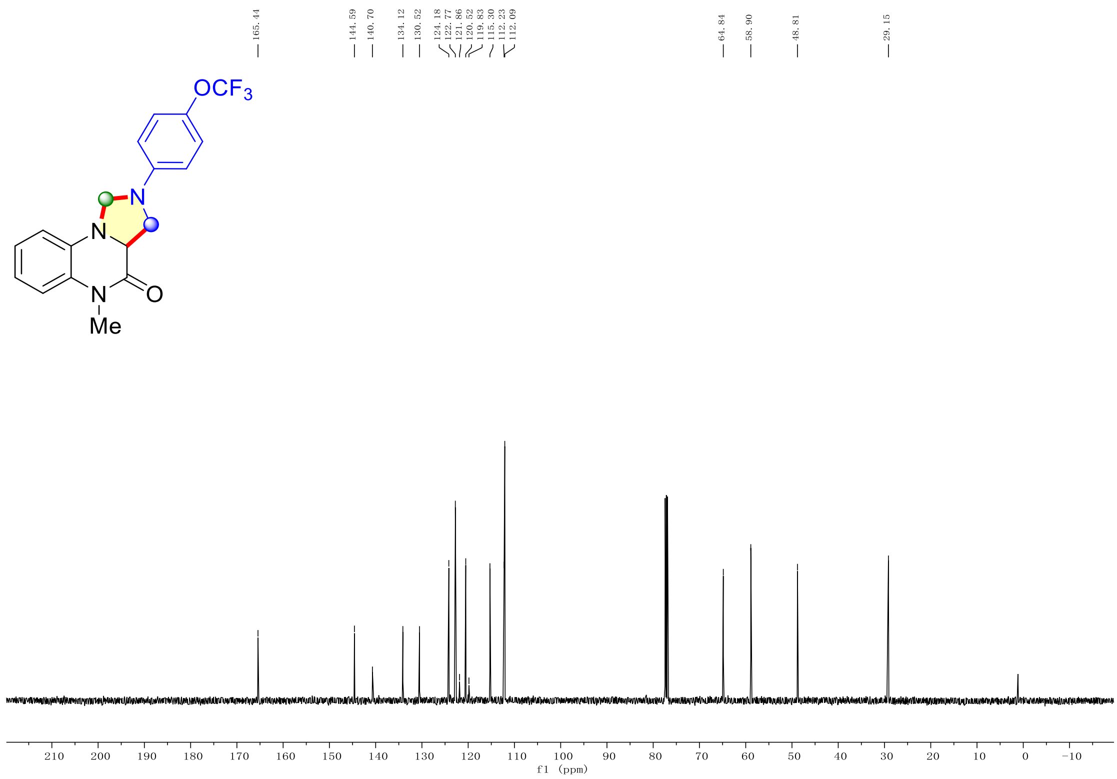


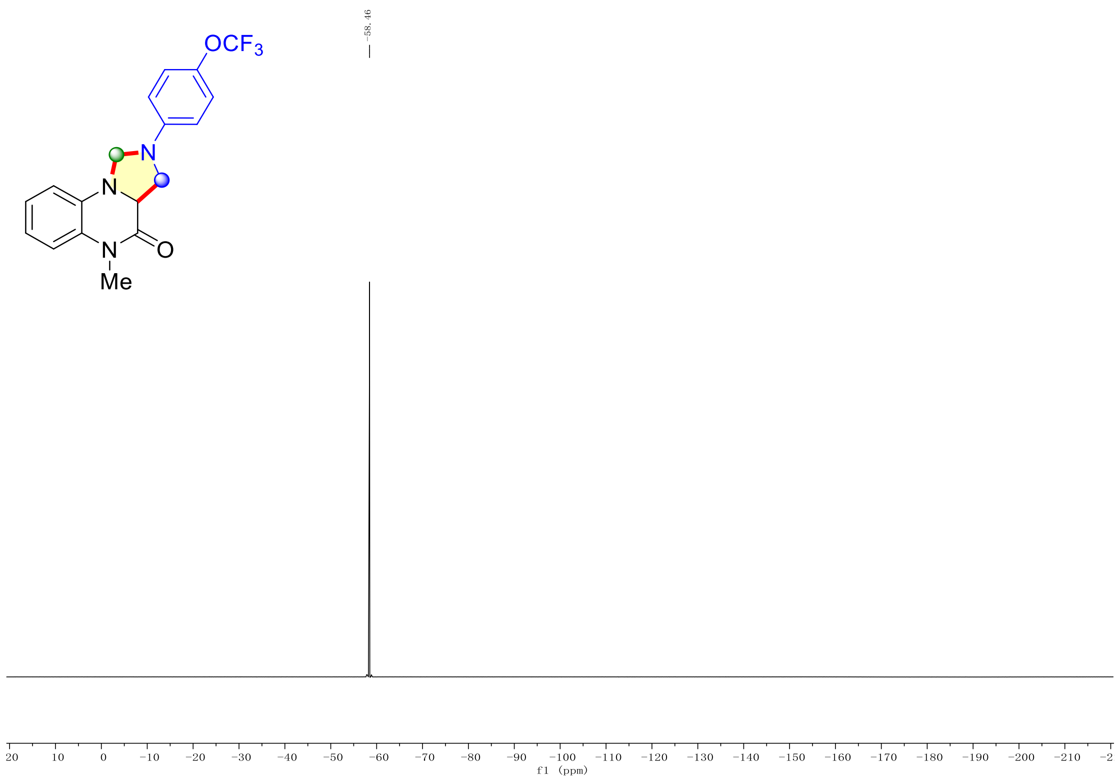


5-methyl-2-(4-(trifluoromethoxy)phenyl)-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4af）

4af ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz) and ^{19}F NMR (471 MHz)

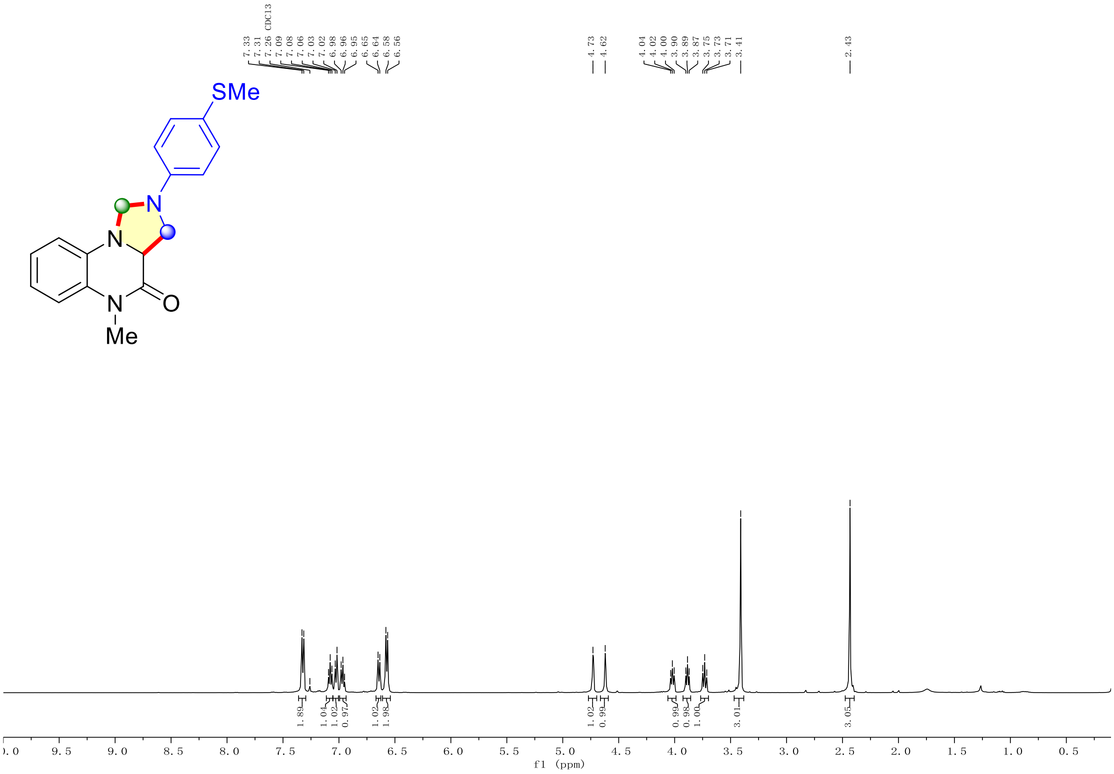


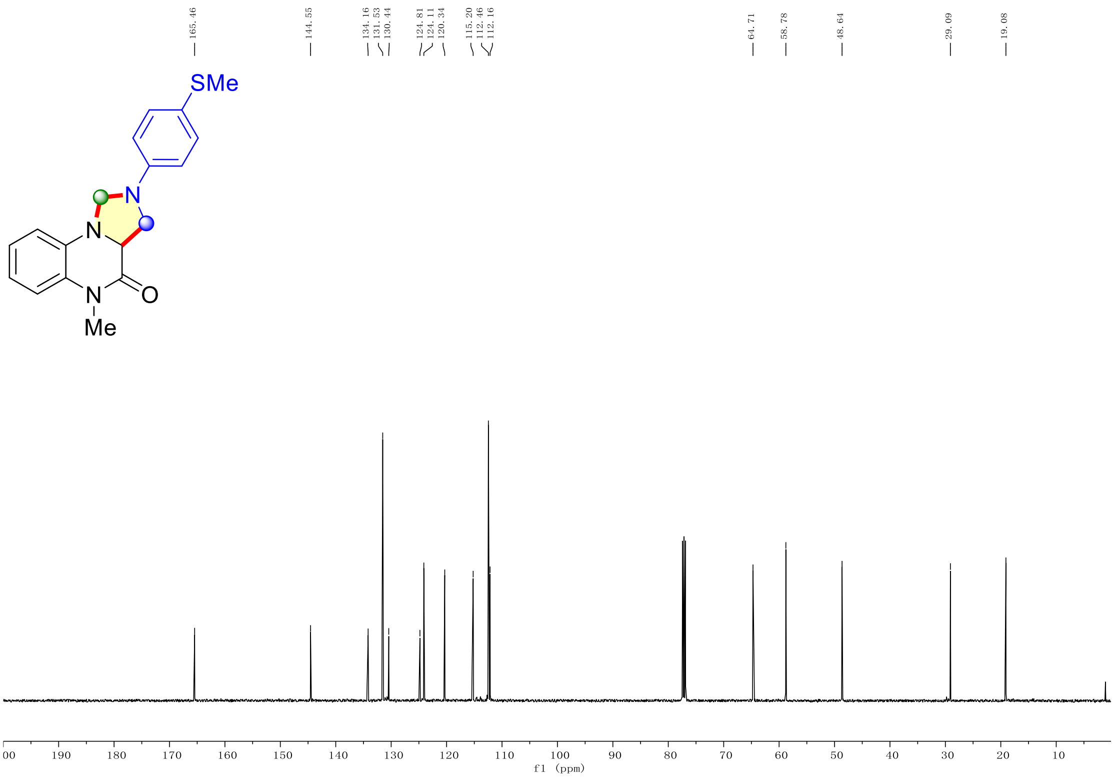




5-methyl-2-(4-(methylthio)phenyl)-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4ag）

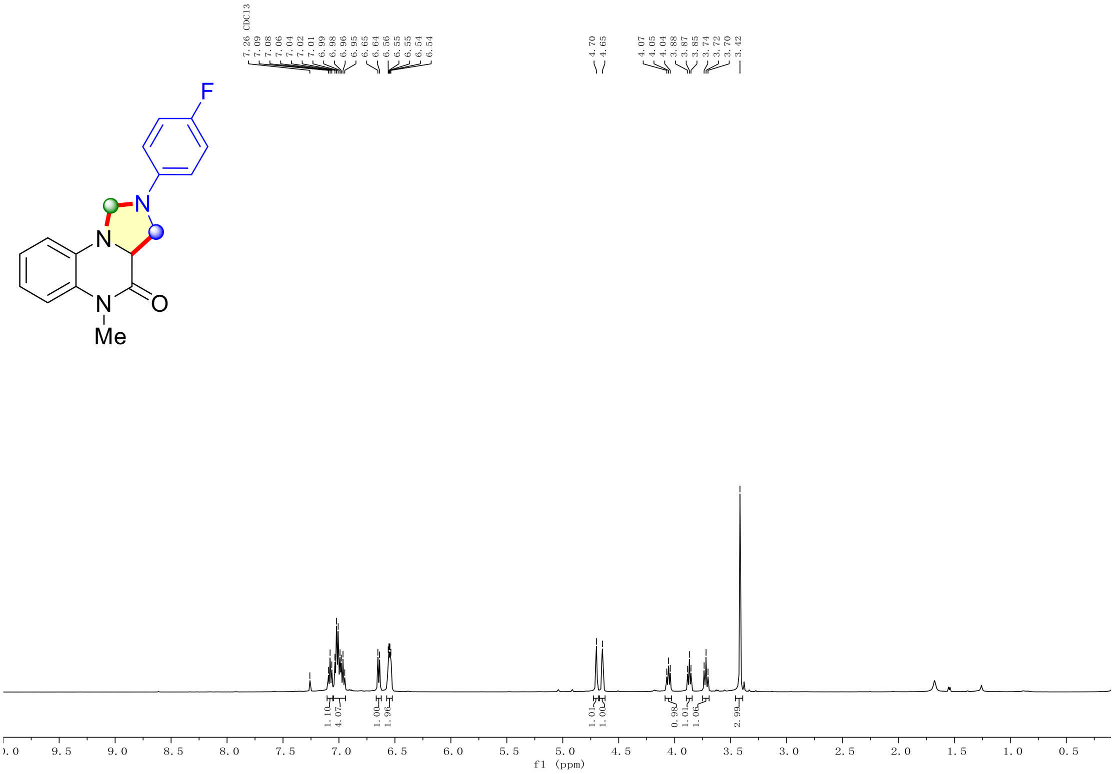
4ag ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)





2-(4-fluorophenyl)-5-methyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4ah）

4ah ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz) and ^{19}F NMR (471 MHz)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7.09
7.08
7.06
7.04
7.02
7.01
6.99
6.98
6.96
6.95
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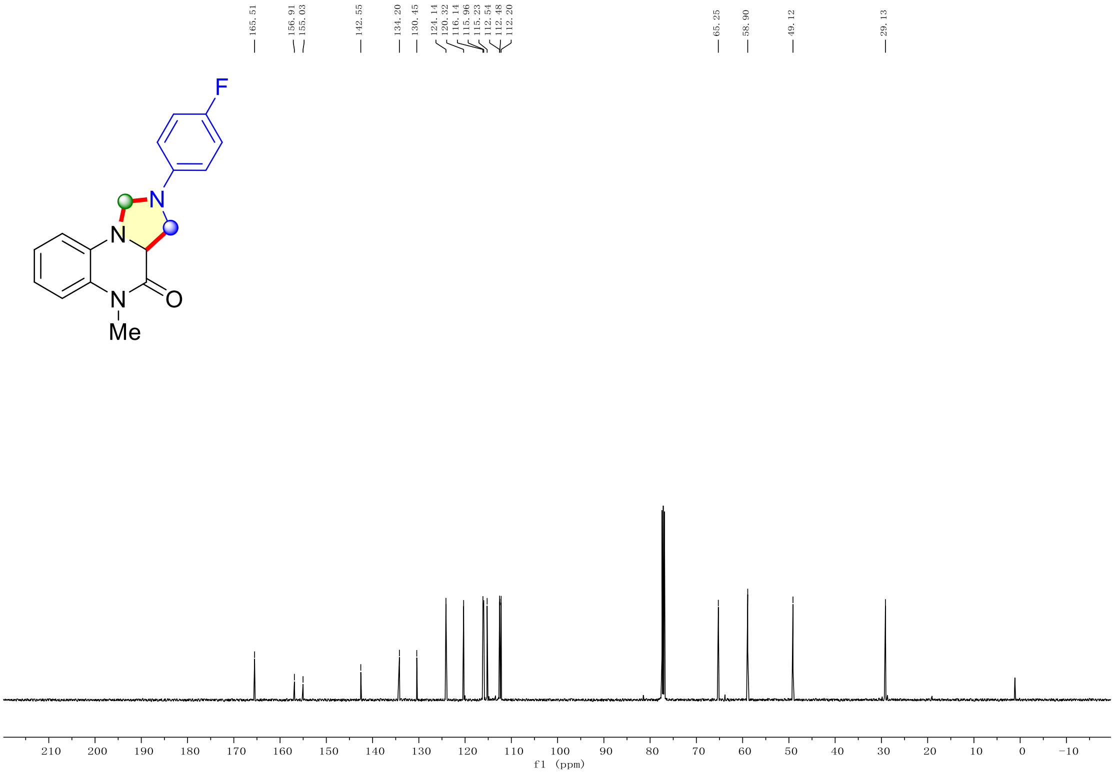
6.64
6.56
6.55
6.54
6.54
4.70
4.65
4.07
4.05
4.04
3.88
3.87
3.85
3.74
3.72
3.70
3.42
F
N
N
N
O
Me
1.10
4.07
1.00
1.96
1.01
1.00
0.98
1.01
1.06
2.99
f1 (ppm)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134.20
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116.14
115.96
115.23
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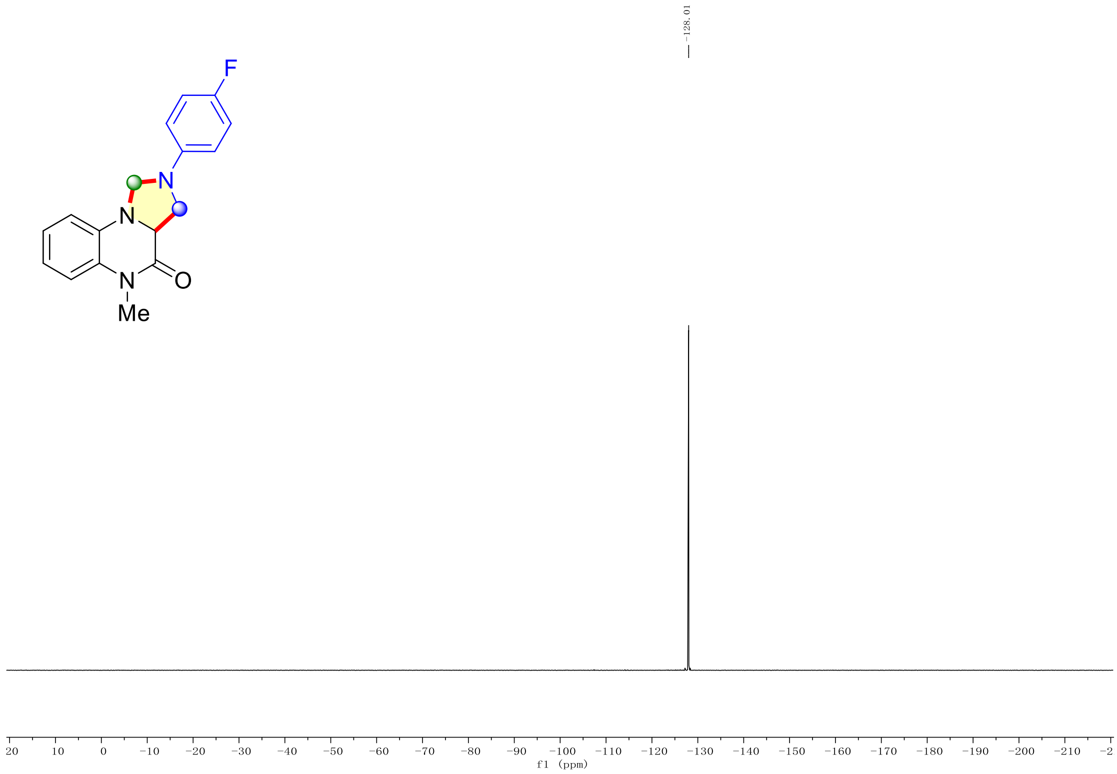
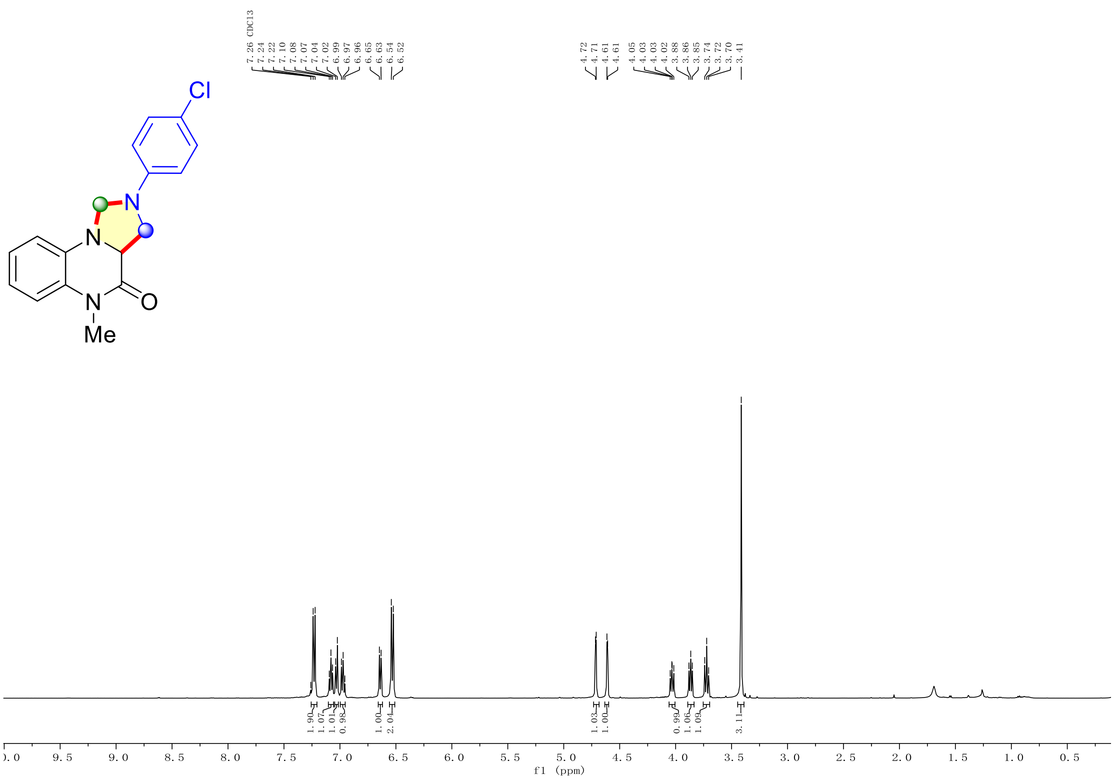
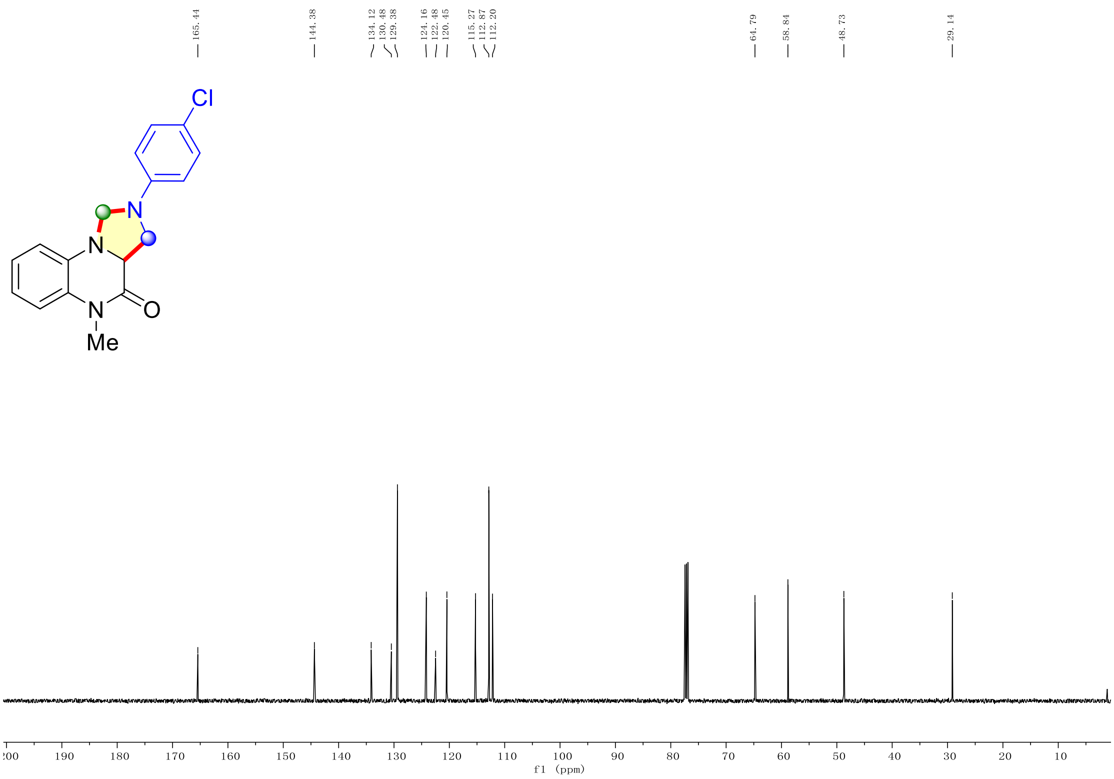
112.20
65.25
58.90
49.12
29.13
F
N
N
N
O
Me
f1 (ppm)



2-(4-chlorophenyl)-5-methyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4ai）

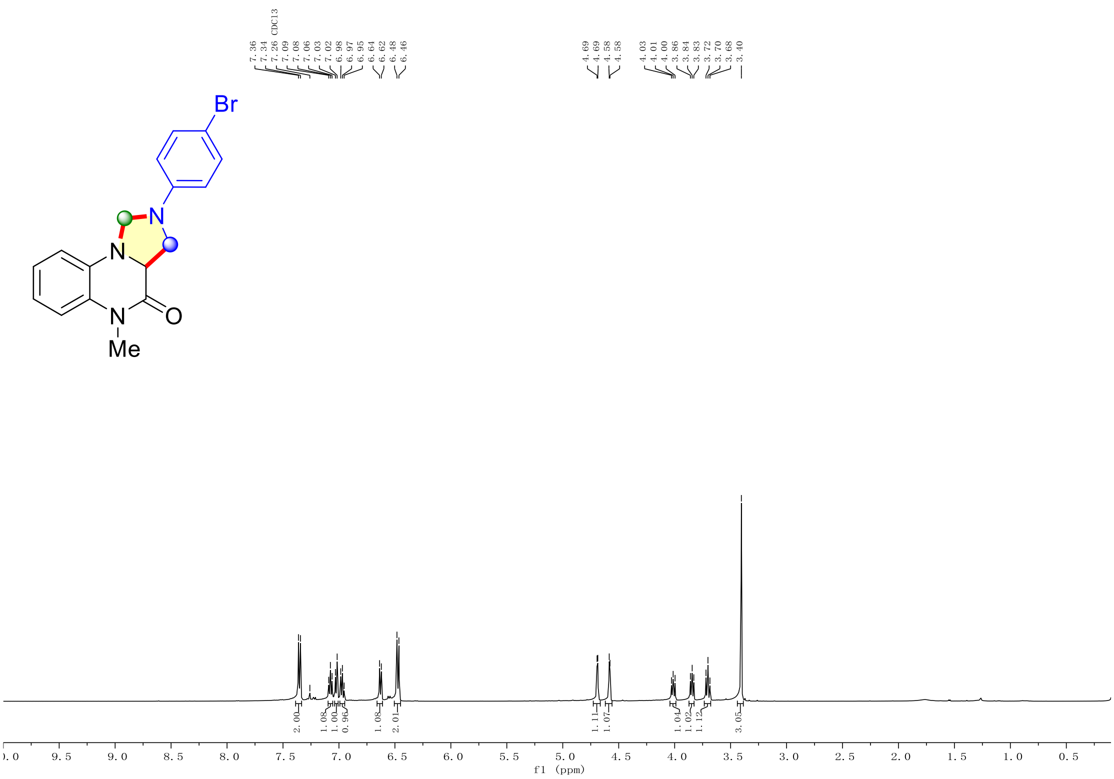
4ai ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

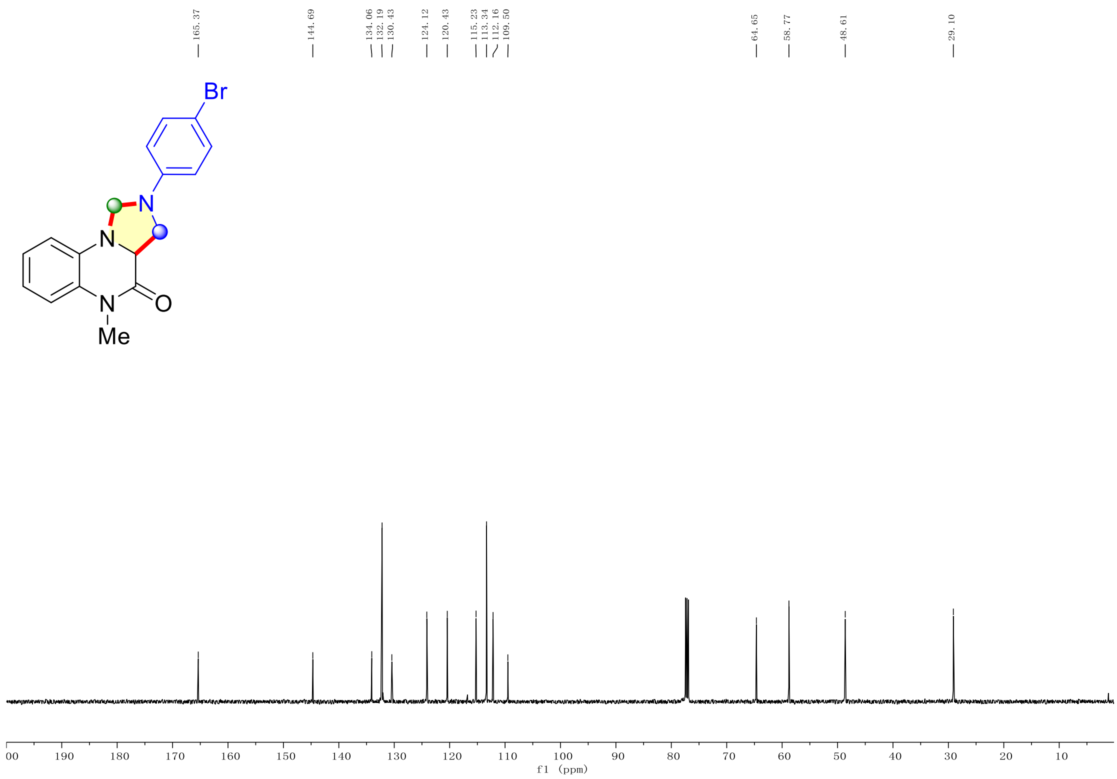




2-(4-bromophenyl)-5-methyl-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4aj）

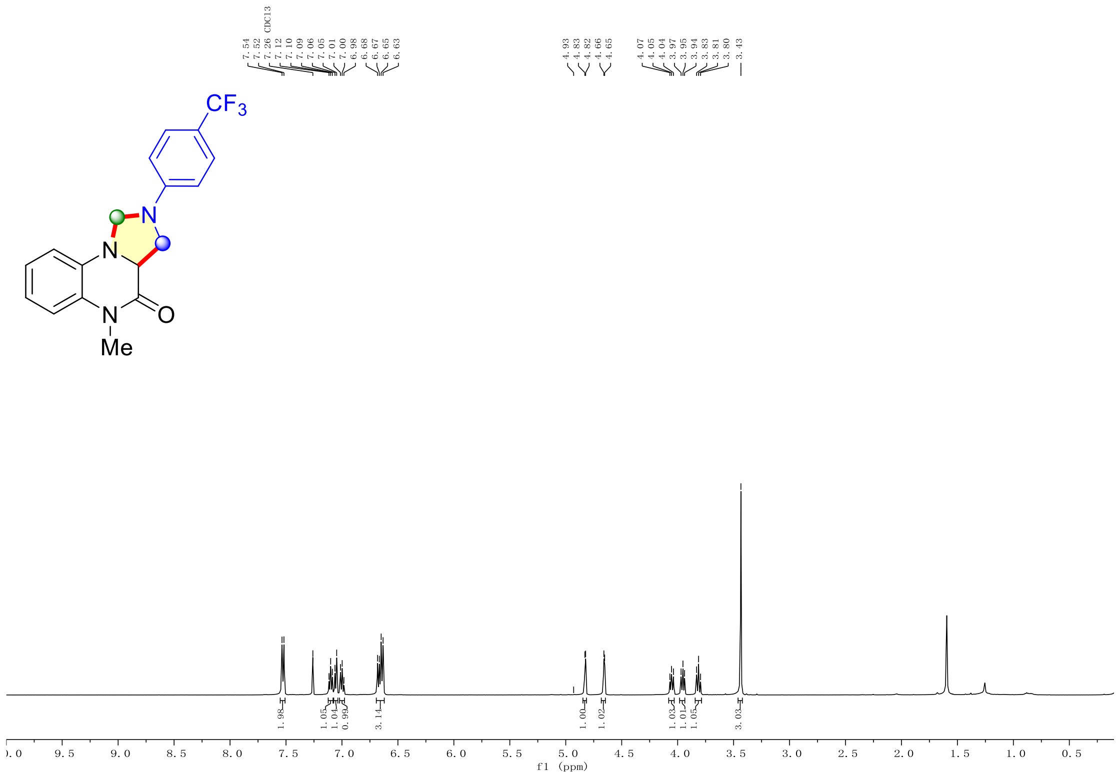
4aj ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)

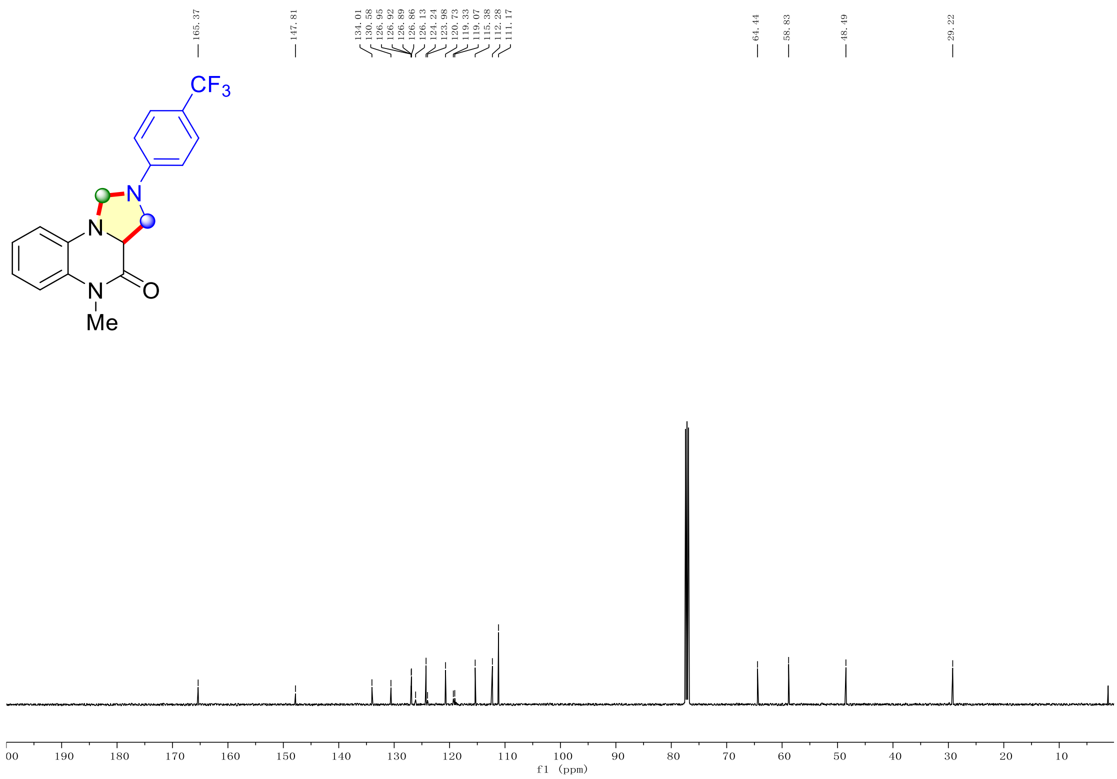


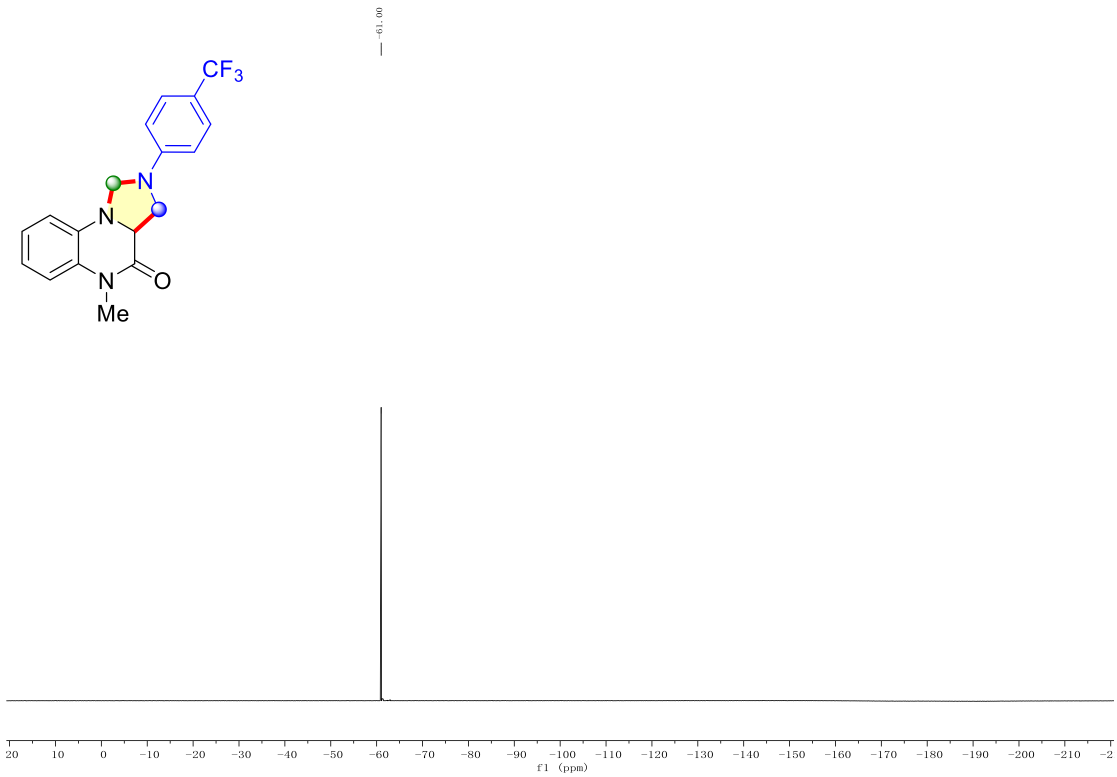


5-methyl-2-(4-(trifluoromethyl)phenyl)-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one（4ak）

4ak ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz) and ^{19}F NMR (471 MHz)

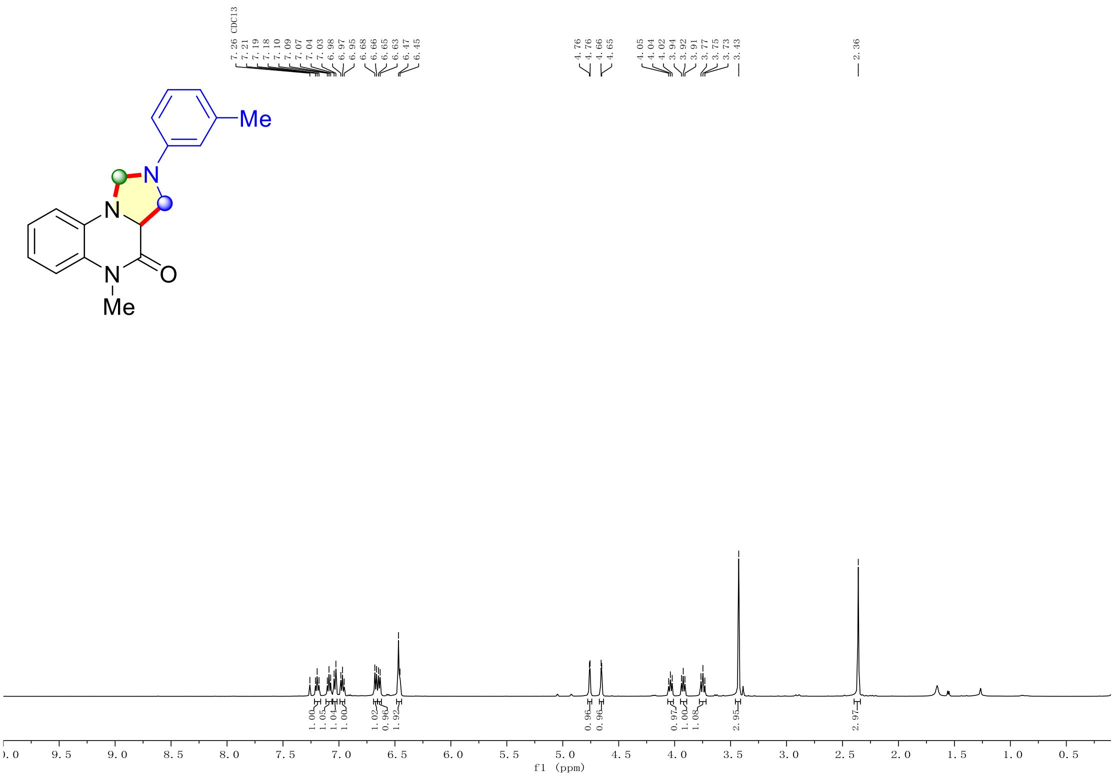


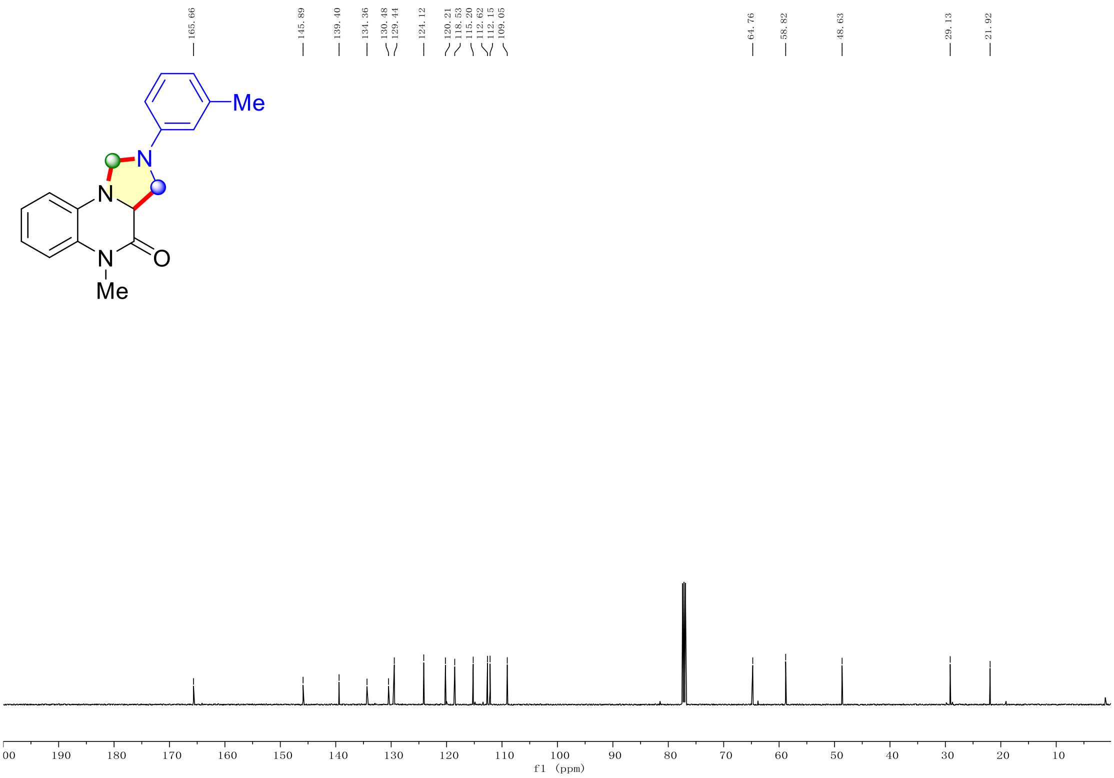




5-methyl-2-(m-tolyl)-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5*H*)-one （4al）

4al ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)





5-methyl-2-(o-tolyl)-1,2,3,3a-tetrahydroimidazo[1,5-a]quinoxalin-4(5H)-one （4am）

4am ^{1}H NMR (500 MHz) and ^{13}C NMR (126 MHz)